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on

Fundamental Studies of Beta Phase Decomposition Modes in Titanium Alloys

by

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30 November 1990

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Fundamental Studies of Beta Phase Decomposition Modes in Titanium Alloys

ABSTRACT

Extensive efforts were made during this grant year to prepare generic overviews on major aspects of phase transformations. Topics on which overviews have been completed or are presently in progress as part of this activity include: crystallographic and mechanistic aspects of growth by shear vs. diffusional growth, interphase boundary structures formed during diffusional transformations in Ti-base alloys, a current summary of the technical bases for three different views of what constitutes bainite, a summary of the diffusionist views on the bainite reaction, the role of ledges in vapor $\rightarrow$ crystal, liquid $\rightarrow$ crystal and crystal $\rightarrow$ crystal phase transformations, a critique of Mats Hillerts' approach to the growth kinetics of diffusional transformations, an assessment of published studies on homogeneous nucleation kinetics in binary metallic alloys and atomic mechanisms of diffusional nucleation and growth. Collaborative research with Dr. M. G. Hall (University of Birmingham) has led (following U. Dahmen, but with differences) to the conclusion that the interphase boundary structure associated with the broad faces of plates formed during non-fcc/hcp transformations should yield a different habit plane when this structure is glissile (as during martensitic growth) than when it is sessile (during diffusional growth). Analysis of published data on ferrite plates formed back-to-back in an Fe-C alloy indicates that the shears associated with these plates are not compensating. Most often, these plates are almost identically oriented, strongly suggesting that sympathetic nucleation is the governing transformation mechanism. Continued TEM studies on the interphase boundary structures assoicated with the (bcc) $\beta \rightarrow$ (hcp) ζ_m massive transformation in a Ag-26 A/O Al alloy have shown that whether the β and ζ_m crystals forming a given interface are Burgers-, Potter- or irrationally orientation-related the structure of the interface is partially coherent. Misfit-compensating ledges (which play no role in growth, and were previously identified at the broad faces of proeutectoid α plates in a hypoeutectoid Ti-Cr alloy by Furuhara, Howe and Aaronson) continue to be the only misfit-compensating defect observed. Growth ledges are present in their usual irregular and erratic fashion, but can play no significant role in the compensation of misfit. Atomic-resolution TEM of these interfaces is now being attempted, in part to ascertain whether or not structural ledges also contribute to the compensation of misfit.

1. INTRODUCTION

From the inception of this program in 1973 (when the P.I. was a faculty member at Michigan Technological University) until the completion of the previous grant year, this program has dealt with proeutectoid, eutectoid and massive transformation mechanisms, usually using binary Ti-base alloys as model systems. In the context of our program on the crystallography and interfacial structures of the massive transformation, inability to retain that portion of the beta matrix which had not transformed to massive alpha because of high M_s temperatures in the several Ti-X systems in which we have discovered a $\beta \rightarrow \alpha_m$ massive transformation (1) has required that this effort be transferred to a Ag-26 A/O Al alloy. In this $\beta \rightarrow \zeta_m$ transformation, a bcc $\rightarrow$ hcp transformation is again operative, indicating that the results obtained are likely to be applicable to the counterpart massive transformations in Ti-X alloys, as this report indeed demonstrates.

During the past grant year and also during the coming grant year, an effort is being made to capitalize upon not only the P.I.'s AFOSR-sponsored research but also upon related fundamental research simultaneously funded by NSF, and for a decade also by ARO, to take a broader view of basic aspects of diffusional phase transformations. The primary thrust of the P.I.'s personal efforts has accordingly been recently devoted to the preparation of "generic overviews". Although the overall directions of these overviews has been determined by the P.I., coincidental receipt of a plethora of invitations to present papers of this type in various contexts has exerted appreciable influence upon the precise manner in which these considerations have been divided amongst the various overviews. Abstracts or summaries of these reviews form the body of the next section.

The experimental research program currently being supported by this grant, on the interphase boundary structures generated during the $\beta \rightarrow \zeta_m$ massive transformation in a Ag-26 A/O Al alloy, is still in progress as a consequence of problems being encountered with performance of atomic resolution TEM studies on this rather difficult alloy. Progress made in the prosecution of this research during the past year is summarized in this report.

With the support of this grant, Dr. Malcolm G. Hall of the University of Birmingham, U.K., spent six weeks in Pittsburgh during the summer of 1990 doing research with the P.I. on fundamental problems associated with the long on-going controversy about the roles of shear and diffusion during the formation of precipitate plates. Appreciable progress was made and further accomplishments are anticipated in next summer's planned research.

2. GENERIC OVERVIEWS ON FUNDAMENTAL ASPECTS OF PHASE TRANSFORMATIONS

2.1 Crystallographic and Mechanistic Aspects of Growth by Shear and by Diffusional Processes

This paper evolved out of an invited talk given during the symposium on "Interface Science and Engineering", presented during the 1988 World Materials Congress and TMS Fall Meeting, held together in Chicago during September, 1988 under the auspices of the ASM-MSD Surfaces and Interfaces Committee and the TMS Electronic Device Materials Committee. The paper with the present title was published in *Metallurgical Transactions A*, 21, (1990), pp. 2369-2409. The paper was authored by H. I. Aaronson, T. Furuhara, J. M. Rigsbee, W. T. Reynolds, Jr. and J. M. Howe.

Growth by shear and by diffusional processes, both taking place predominantly by means of ledge mechanisms, are reviewed for the purpose of distinguishing critically between them at the atomic, microscopic and macroscopic levels. At the atomic level, diffusional growth is described as individual, poorly coordinated, thermally activated jumps occurring in the manner of biased random walk, whereas growth by shear is taken to be tightly coordinated "glide" of atoms to sites in the product phase which are "predestined" to within the radius of a shuffle. Obedience to the invariant plane strain surface relief effect and the transformation crystallography prescribed by the phenomenological theory of martensite is shown to be an unsatisfactory means for distinguishing between these two fundamentally different atomic growth mechanisms. In substitutional alloys, continuous differences in composition and in long-range order from the earliest stages of growth onwards are concluded to be the most useful phenomenological approach to achieving differentiation. At a more fundamental level, however, the details of interphase boundary structure are the primary determinant of the operative mechanism (when the driving force for growth is sufficient to permit either to occur). In the presence of a stacking sequence change across the boundary, terraces of ledges are immobile irrespective of their structural details during diffusional growth. Kinks on the risers of superledges are probably the primary sites for diffusional transfer of atoms across interphase boundaries. In martensitic transformations, on the other hand, terraces containing edge dislocations in glide orientation or pure screw dislocations are mobile and accomplish the lattice invariant deformation, though probably only after being overrun by a transformation dislocation. Risers associated with transformation dislocations are also mobile and cause the crystal structure change during growth by shear. The successes achieved by the invariant line component of the phenomenological theory of martensite in predicting precipitate needle growth directions and precipitate plate habit planes (Dahmen et al) are here ascribed to the rate of ledge formation usually being a minimum at an interface containing an invariant line, primarily because nuclei formed sympathetically at this boundary orientation are likely to have the highest edge energies. Since martensite plate broad faces also contain the invariant line, the ability of the phenomenological theory to predict the habit plane and the orientation relationships of both precipitate and martensite plates is no longer surprising. The invariant plane strain relief effect at a free surface can be generated by precipitate plates when growth ledges are generated predominantly on only one broad face and only one of several crystallographically equivalent Burgers vectors of growth ledges is operative. Both preferences probably result from larger reductions in transformation strain energy for the particular geometry with which a given plate intercepts the free surface. Precipitate morphology often differs significantly from that of martensite even if precipitates are plate-shaped, and can readily differ very greatly. Whereas martensite morphology is determined by the need to minimize shear strain energy, that of precipitates derives from the more flexible base of the interphase boundary orientation-dependence of the reciprocal of the average inter-growth ledge spacing, as modified by both the orientation-dependence of inter-kink spacing on growth ledge risers and the spacing/height ratio-dependence of diffusion field overlap upon growth kinetics.

2.2 Interphase Boundary Structures Associated with Diffusional Phase Transformations in Ti-Base Alloys

This paper is based upon an invited talk given during the symposium on "Interfaces and Surfaces of Titanium Materials", presented during the 1988 World Materials Congress and TMS Fall Meeting in Chicago during September, 1988 under the auspices of the TMS Titanium Committee. The paper with the present title was published in Metallurgical Transactions A, 21, (1990), pp. 1627-1643. This paper was authored by T. Furuhara and H. I. Aaronson.

Interphase boundary structures generated during diffusional transformations in Ti-base alloys, especially the proeutectoid α and eutectoid reactions in a β-phase matrix, are reviewed. Partially coherent boundaries are shown to be present whether the orientation relationship between precipitate and matrix phases is rational or irrational. Usually, these structures include both misfit dislocations and growth ledges. However, grain boundary α allotriomorphs (GBA's) do not appear to develop misfit dislocations at partially coherent boundaries. Evidently, these dislocations can be replaced by ledges which provide a strain vector in the plane of the interphase boundary. The bainite reaction in Ti-X alloys produces a mixture of eutectoid α and eutectoid intermetallic compound. Both eutectoid phases are partially coherent with the β matrix, and both grow by means of the ledge mechanism, though unlike pearlite the ledge systems of the two phases are structurally independent. Even after deformation and recrystallization, the boundaries between the eutectoid phases and the β matrix, as well as between these phases, are partially coherent. Titanium and zirconium hydrides have partially coherent interphase boundaries with respect to their β matrix. The recent observation of ledgewise growth of γ TiH with *in situ* high-resolution transmission electron microscopy (HRTEM) suggests that, repeated suggestions to the contrary, these hydrides do not grow by means of shear transport of Ti atoms at rates paced by hydrogen diffusion.

2.3 Bainite Viewed Three Different Ways

This paper is based upon the invited introductory lecture for the "International Conference on Bainite", presented during the 1988 World Materials Congress and TMS Fall Meeting in Chicago during September, 1988 under the auspices of the ASM International Phase Transformations Committee and the TMS Ferrous Metallurgy Committee. The paper with the present title was published in Metallurgical Transactions A, 21, (1990), pp. 1343-1380. The paper was authored by H. I. Aaronson, W. T. Reynolds, Jr., G. J. Shiflet and G. Spanos.

The present status of the three principal definitions of bainite currently in use is reviewed. On the surface relief definition, bainite consists of precipitate plates producing an invariant plane strain surface relief effect which form by shear, i.e., martensitically, at temperatures usually above M_s and M_d. The generalized microstructural definition describes bainite as the product of the diffusional, non-cooperative, competitive ledgewise growth of two precipitate phases formed during eutectoid decomposition, with the minority phase appearing in non-lamellar form. This alternative mode of eutectoid decomposition is thus fundamentally different from the diffusional, cooperative, shared-growth-ledges mechanism for the formation of pearlite developed by

Hackney and Shiflet. The overall reaction kinetics definition of bainite views this transformation as being confined to a temperature range well below that of the eutectoid temperature and being increasingly incomplete as its upper limiting temperature, the kinetic-B_s, is approached. Recent research has shown that, even in steels (the only alloys in which this set of phenomena has been reported), incomplete transformation is not generally operative. Revisions in and additions to the phenomenology of bainite defined in this manner have been recently made. Extensive conflicts amongst the three definitions are readily demonstrated. Arguments are developed in favor of preference for the generalized microstructural definition, reassessment of the overall reaction kinetics definition and discarding of the surface relief definition.

2.4 A Summary of the Present Diffusionist Views on Bainite

This paper is scheduled to be prepared during January and February, 1991; it has been invited for contribution to a special issue of the Materials Transactions of the Japan Institute of Metals (to be published entirely in English), intended to be devoted wholly to bainitic transformations. This paper will be authored by H. I. Aaronson, W. T. Reynolds, Jr. and G. Spanos. The subject matter to be covered will be mainly a compact summary of the lengthy overview papers described in items 2.1 and 2.3. Inasmuch as only six pages in the Japanese journal will be provided, however, a considerable feat of condensation will be required in order to present our views on these matters in sufficient detail for them to be intelligible on a "stand-alone" basis.

2.5 The Role of Ledges in Vapor → Crystal, Liquid → Crystal and Crystal → Crystal Phase Transformations

This paper, which is still being written, is based upon an invited talk given during the symposium titled "The Role of Ledges in Phase Transformations" presented during the 1989 TMS-ASM Fall Meeting in Indianapolis, IN during October, 1989 under the auspices of the ASM Phase Transformations Committee. The paper will be published, after review, in Metallurgical Transactions A; it will be authored by H. I. Aaronson and T. Furuhara.

Although preparation of this paper has been in progress, off and on, for about one year, the first draft has yet to be completed. As this paper has evolved, it has become an effort designed to encompass an immense range of theory and of experimental observations on crystal growth from the vapor, liquid and solid phases. The scope of this effort has become so large that the status of paper 2.2 in this outline as the longest published to date in Metallurgical

Transactions will almost surely be overthrown by this paper! However, this unexpectedly large effort is turning out to be quite rewarding, as theory and/or experiment in one area proves to be extensively applicable in another, despite the fact that only one of the three "matrix phases" being considered is crystalline, or even solid. In other instances, marked differences in behavior appear--which previous workers have failed to apprehend, and as a result have inappropriately transferred explanations from one area to another. Sorting out the fundamentals of these similarities and differences is truly a most pleasant task. The major similarity among the three to which the P.I. wishes to draw attention is the erraticity of ledgewise growth in all three types of transformation. Identification of such behavior is best done by photographing growth in situ. Most of the P.I.'s efforts in this area were part of collaborative research with Drs. K. R. Kinsman and C. Laird when all three of us were staff members of the Scientific Laboratory of Ford Motor Co. The P.I. has continued to urge the importance of these results ever since. Within the last decade or so, the significance of this work has begun to be appreciated by critics, and as a result attempts are being made more frequently now to attack the validity of these results. In preparing this overview it has been most fortifying to find that our results on crystal → crystal transformations actually amount, in the large, to reproduction in a different medium of well documented data on the growth of inorganic crystals in aqueous media reported 40 or more years ago.

2.6 On the Approach of Mats Hillert to the Growth Kinetics of Diffusional Phase Transformations

This paper is based on an invited talk given during "The Mats Hillert Symposium in Materials Science: Formation of Microstructures", held in Stockholm, Sweden on October 22 and 23, 1990 in honor of Prof. Hillert's forthcoming retirement. This paper has been completed and will be published as part of a special issue of the Scandanavian Journal of Metallurgy. The paper is authored by H. I. Aaronson, T. Furuhara and M. Enomoto.

The Hillert approach to analysis of growth kinetics assumes that interphase boundaries are disordered and thus normally offer negligible resistance to growth. An evaluation of the present status of this assumption is made upon two bases. The first utilizes growth kinetics data taken at low enough resolutions in space and time so that the role of ledges is not directly detectable. The second basis examines interfacial structure as well as growth kinetics, at resolutions sufficient to observe ledges and to evaluate their role during growth. Lengthening and thickening of plates and of grain boundary allotriomorphs, growth kinetics of massive transformations and edgewise growth of pearlite are considered upon both bases. On the first, the disordered boundary assumption usually works well. While on the second basis the interphase boundary structure has now been shown to be partially coherent during all of these processes, as long as growth ledges are closely spaced the disordered boundary assumption often remains a useful approximation.

2.7 An Assessment of Studies on Homogeneous Nucleation Kinetics in Binary Metallic Alloys

This paper, whose writing is nearly complete, is based upon an invited talk given during the symposium titled "The G. Marshall Pound Memorial Symposium on the Kinetics of Phase Transformations", presented during the 1990 TMS-ASM Fall Meeting in Detroit, MI during October, 1990 under the auspices of the ASM Phase Transformations Committee. This paper will be published, after review, in Metallurgical Transactions A; it will be authored by H. I. Aaronson and F. K. LeGoues.

Since growth rather than nucleation has been the primary focus of research performed under the sponsorship of this grant, some introductory material appears appropriate. The thermodynamic essence of nucleation theory was formulated by J. Willard Gibbs in 1887 (2). The kinetic component of the theory was largely developed from the 1920's through the 1940's, mainly in Europe. Despite its Gibbsian base, this theory has long been the subject of serious controversies. Experimental testing of nucleation theory--restricted to homogeneous nucleation in order to avoid the still greater complexities of heterogeneous nucleation--was first done with sufficient completeness in the 1960's and 1970's. Most of these experiments measured the nucleation kinetics of one liquid phase within another. Each such study yielded results markedly in disagreement with nucleation theory, causing serious doubts to be broadcast about the essential correctness of the theory. Binder and Stauffer (3) were the first to recognize that the "cloud chamber" experiments used to evaluate nucleation kinetics had been incorrectly analyzed. What experimentalists had taken to be direct estimates of the undercooling needed to produce detectable nucleation rates were actually studies of a complex melange of nucleation, growth and coarsening. This lead was followed up in more detail by Langer and Schwartz (4), who concluded: (a) with the possible exception of a single data point, there is no disagreement between any of these experiments and the theory, and (b) experiments involving growth and coarsening as well as nucleation are too insensitive to nucleation kinetics to permit a reliable test to be made of nucleation theory.

Experimental studies designed to test quantitatively solid $\rightarrow$ solid nucleation theory in metallic alloys began with the work of Servi and Turnbull (5) in 1966 and continued with three investigations by Kirkwood and co-workers (6-8) from 1970 - 1977. Although all four papers reported agreement with the theory, the data reported by Servi and Turnbull were based on electrical resistivity measurements, followed up by a complex four-layer analysis, while the TEM measurements of Kirkwood et al were clearly studies focussing far more on coarsening than on nucleation. LeGoues and Aaronson (9) made a study on three Cu-Co alloys, reported in 1984, which did yield reliable data on the kinetics of homogeneous nucleation, uncontaminated by coarsening. They achieved these results by recognizing that the experiments must be conducted within a "nucleation window" of alloy composition-reaction temperature-reaction time if coarsening effects are to be avoided. They also showed that their data supported classical, Cahn-Hilliard (10) continuum non-classical and Cook-DeFontaine (11,12) discrete lattice point non-classical versions of nucleation theory.

During the 1980's a number of investigations of nucleation kinetics, using more elaborate techniques such as field ion microscope/atom probe and small-angle neutron scattering, were reported by West German groups under the leadership of Haasen (13). Several of these studies again led to the conclusion that nucleation theory (mainly the classical theory) is in error. In this review, we examine all available data on solid $\rightarrow$ solid nucleation kinetics in metallic alloys and conclude that only the LeGoues-Aaronson data are both valid and clear-cut (though at a composition used by these workers and Servi and Turnbull, the two data sets were virtually indistinguishable, thereby validating the latter data). Just as did Langer and Schwartz earlier, we conclude that disagreements alleged between theory and experiment derive in part or in whole from the presence of simultaneous coarsening.

2.8 Atomic Mechanisms of Diffusional Nucleation and Growth

This paper, yet to be written, will be based upon the Institute of Metals Lecture, given by the P.I. at the TMS Annual Meeting in Anaheim, CA in February, 1990. The paper will be published in Metallurgical Transactions A. The following is the abstract of this talk, as published in the program for the Anaheim Meeting.

This lecture will be based upon ideas developed from Dr. R. F. Mehl's demonstration, in a series of papers entitled "Studies upon the Widmanstatten Structure", published between 1931 and 1937, that the broad faces of precipitate plates are formed by particularly well matched conjugate habit planes in the matrix and precipitate phases. The point will first be made that purely diffusional nucleation processes can lead reproducibly to the lattice orientation relationships which make Widmanstatten morphologies possible. Confirmation of the essential correctness of nucleation theory by recent experiments on Cu-Co alloys provides a firm base for this and all further considerations. Differences in the nucleation mechanics of martensitic and diffusional transformations will be shown to lead simply and directly to sharp differences in both the kinetics with which misfit dislocations are acquired and their orientations with respect to interphase boundaries. These differences will be seen to lead in turn to the drastically different shear (= martensitic) and diffusional mechanisms of growth. The unit atomic process in growth by shear is the tightly coordinated "gliding", through dislocation motion, of successive atoms across advancing partially coherent interphase boundaries. In diffusional growth, however, this process is the loosely coordinated, biased random walk, diffusional jumping of individual atoms across the risers of growth ledges, or kinks on these risers, through regions containing sufficient local atomic disorder to make such jumps energetically feasible. Both types of growth are shown to be capable of satisfying the invariant-plane-strain surface relief effect and the crystallographic requirements and consequences of the phenomenological theory of martensite crystallography. Only "derivative" requirements of this theory, including absence of changes in composition and in long-range order, availability of sufficient driving force and the presence of an appropriate interphase boundary structure are capable of distinguishing between these two different growth mechanisms--and then only when all are simultaneously employed. The importance of growth ledges in diffusional transformations will be particularly emphasized through examples including the thickening of grain boundary allotriomorphs, the degeneration of the Widmanstatten ferrite morphology and the slowing down of ferrite growth through action of the solute drag-like effect, and both bainitic and pearlitic modes of eutectoid decomposition.

3. COLLABORATIVE RESEARCH WITH DR. M. G. HALL ON FUNDAMENTAL TRANSFORMATION MECHANISMS

3.1 Introduction

Dr. Malcolm G. Hall, who is associated with the School of Metallurgy and Materials at the

University of Birmingham, U.K., worked with the P.I. while both were at the Scientific Laboratory of Ford Motor Co. 20 years ago. He joined the University of Birmingham staff at about the time the P.I. departed Ford for Michigan Technological University. Since then, Dr. Hall and the P.I. have periodically worked together, both through the mails and by means of personal visits Dr. Hall paid to Michigan Tech and later to Carnegie Mellon University. These interactions have results in a considerable number of publications, some of which have made significant impacts upon the technical literature. Dr. Hall invented the concept of (misfit-compensating) structural ledges while at Ford, and since then has published, as part of this continuing collaboration, important O-lattice analyses and TEM studies of fcc:bcc interfaces. Nearly all of our joint work has revolved around the problem which lies at the heart of the present grant, i.e., understanding the crystallographic, surface relief and interfacial structure differences between diffusional and martensitic mechanisms of forming plate-shaped transformation products.

Dr. Hall visited CMU for six weeks during the summer of 1990 with the support of this grant, his department at the University of Birmingham and also personal funds from both sides. Although we had originally planned that this visit would focus upon the origins of tent-shaped surface relief effects, two other projects were given priority instead. The surface relief study will be re-addressed next summer and will be the subject of an invited talk Dr. Hall will give at the Pacific Rim Countries Conference on the Roles of Shear and Diffusional Growth in the Formation of Plates in Crystalline Solids during December, 1992, in Hawaii, as described in section 4 of this Report.

3.2 Effects of the Interfacial Structure Differences Associated with Shear and Diffusional Growth upon the Habit Plane of Plates

During fcc $\rightarrow$ hcp transformations in which growth takes place by a shear mechanism, only a Bain strain is required. Neither a lattice invariant deformation nor a rigid body rotation is needed or is present (14). Thus during both martensitic and diffusional growth, this transformation requires only the lateral motion of ledges bounded by $\underline{a}/6\langle 112\rangle$ Shockley partial dislocations. While the atomic mechanism through which these Shockley partial ledges accomplish the growth process differs sharply during the two types of growth, involving tightly coordinated glide-type motion of atoms across kinks in the risers of advancing ledges during shear, and thermally activated diffusional jumps across kinks proceeding in the style of biased random walk during diffusional growth, at the resolution levels of "ordinary" TEM down through that of optical microscopy the products of shear and diffusional growth are indistinguishable during fcc/hcp transformations. They have the same orientation relationship and habit plane and produce the same surface relief effect.

For fcc $\rightarrow$ bcc, bcc $\rightarrow$ hcp and other crystal structure changes, on the other hand, both a lattice invariant deformation and a rigid body rotation are required. The former, now abbreviated as LID, is accomplished by means of unit lattice vector or "total" misfit dislocations, located in the conjugate atomic habit planes which form the terraces of ledged interfaces. The Burgers vector of these dislocations must lie at an angle to the atomic habit planes (14) in order to permit these dislocations to glide back into the interface (and thus accomplish the LID) after they have been overrun by the (partial) transformation dislocations which form the risers of these interfaces (15).

During diffusional growth, on the other hand, the Burgers vector of these dislocations lies within the atomic habit planes, thereby preventing them from gliding and accomplishing the LID during growth. Alternatively, they can be immobilized by the presence of two sets of misfit dislocations in the interface whose Burgers vectors are oriented so that they must glide in different directions. If structural ledges (16) or misfit-compensating ledges (17) replace one or both sets of misfit dislocations, the terraces of a ledges interphase boundary will also be immobilized with respect to shear, though for different (16,17) reasons. In the case of diffusional growth, whether the terraces (one of which can, in principal, encompass an entire interface such as a broad face or an edge of a precipitate plate) are fully coherent or partially coherent, and whether the dislocations on the terraces are in glissile or in sessile orientation, the immobility of the coherent regions between misfit dislocations immobilizes the entire boundary. This situation occurs because changing the stacking sequence diffusionally requires insertion of substitutional atoms into temporarily interstitial sites at closely packed interfaces, a kinetically infeasible process (18).

The question now arises as to the effect of the difference in the orientation of the Burgers vector of the misfit/LID dislocations in the terraces during shear with respect to that during diffusional growth upon the macroscopic habit plane of the interface. Fig. 1, reproduced from a seminal paper by U. Dahmen (19), is a cut-away view of a partially coherent interface which could subsist at an fcc:bcc or a bcc:hcp boundary. The vector $\underline{u}$ is parallel to the invariant line of the transformation, along which mismatch is zero. Since this vector usually lies in directions which are irrational in one or both lattices, the invariant line interface "breaks down" into a stepped or ledged interface (19). The ledges whose apparent habit plane (connecting the riser/terrace intersections of successive ledges) is parallel to $\underline{u}$ are the structural ledges independently discovered by Hall et al (16). Also shown in this interface are two glissilely oriented LID dislocations. Dahmen claims that their out-of-the-terrace Burgers fector gives rise to a second set of structural ledges parallel to the vector $\underline{v}$.

During this study, we have considered the validity of introducing this second set of ledges. Our first conclusion is that they cannot be structural ledges. There can be only one invariant line for a given pair of crystal structures with a particular orientation relationship between them (20). Hence there can be only one set of structural ledges. The second set of ledges still exists. However, this set does not perform a misfit-compensating function (as do structural ledges); it is, instead, merely a "geometrically necessary" consequence of the Burgers vector component orthogonal to the terrace plane.

Irrespective, though, of the interpretation placed upon the "second" set of ledges, whose apparent habit plane is parallel to $\underline{v}$, we now recognize that the apparent or macroscopic habit plane of this interface has been rotated away from the apparent habit plane which obtains when the Burgers vector of the misfit/LID dislocations is parallel to the terrace plane and thus only structural ledges are present. Using the Nishiyama-Wassermann (21,22) orientation relationship between fcc and bcc crystals as an illustrative example, the Burgers vector of a/2<011> dislocations lies in the terraces of the structural leges, resulting in a sessile interfacial structure. However, if the Burgers vector is instead a/2<101> or a/2<110>, a component of the Burgers vector lies out of the terrace plane of the structural ledges and the habit plane is rotated through an angle given by tan $\Theta = 0.3/1.23$, or 9.2° away from the habit plane of the sessile interface (where 1.23 nm is the spacing between parallel dislocations).

We have previously made a considerable effort to collect crystallographic and other data on precipitate plates which disagree with the predictions of the phenomenological theory of martensite crystallography (PTMC) (15,18,23), and have used this as empirical evidence of the inapplicability of the theory to diffusional transformations. On the present considerations, we now have the more useful possibility of connecting differences in the macroscopic habit plane of precipitate plates relative to those predicted by the PTMC with differences in the interfacial structure of the broad faces of these two types of plate-shaped transformation product. A detailed examination of literature on the habit plane of ferrite and bainite plates in steel, and then of plates formed during other crystal structure changes, has therefore been planned in order to attempt this rationalization. Success in achieving such a correlation between habit plane and interfacial structure differences would provide strong support for our view that only martensite plates (with very few possible exceptions) can and do grow by means of the shear mechanism at the atomic level.

A second point to be noticed in Fig. 1 is that glissilely oriented misfit/LID dislocations on the terraces of the structural ledges compensate lattice misfit across the terraces in less than optimum fashion. Taking the inter-dislocation spacing across the aforementioned Nishiyama-Wassermann interface to be 2.46 nm when $\underline{b}$ = a/2<011>, as can be appropriate for fcc:bcc interfaces in several alloy systems, the other two Burgers vectors require that this spacing be reduced to 1.23 nm. In principle, this provides another means of distinguishing between glissile and sessile interphase boundaries. However, it has long been established that unless precipitates are held at the temperature where they formed for long times the inter-dislocation spacing at their interfaces are often considerably greated than those which would obtain at optimum compensation of mismatch (18). Hence this criterion must be used with caution.

The other three formal crystallographic components of the PTMC will now be briefly considered from the present viewpoint. The orientation relationship for shear and diffusional transformations could be identical, with differences occurring only in the (macroscopic) habit plane. However, Wayman (24) has tabulated a large quantity of very accurate OR data for martensite plates formed in steel and has demonstrated conclusively that these relationships are invariably at least slightly irrational. During diffusional transformations, however, rational relationships tend to prevail. This point must thus be examined further in the present context. So, also, must be the shape strains (the generalization of the surface relief effect) associated with the two types of interfacial structure. In respect of structural evidence for the operation of a lattice invariant deformation, there should be none when the LID dislocations are total dislocations in both lattices. However, when they are partial dislocations in the product phase lattice, either stacking faults or twins will be left behand in the plates produced by the transformation (25). Hence the presence of such defects in martensite but not in precipitate plates in a given alloy in which both types of transformation can occur should constitute strong evidence for a diffusional mode of growth of the precipitates.

3.3 Are Pairs of Ferrite Plates Formed Back-to-Back Characterized by Compensating Shears?

In his paper in the 1968 Symposium on The Mechanism of Phase Transformations in Crystalline Solids, held at the University of Manchester, the P.I. presented an optical micrograph showing a pronouncedly tent-shaped surface relief effect associated with a single ferrite sideplate (26). Srinivasan and Wayman (27) objected to this observation, claiming that it must have resulted from the formation of two sideplates back-to-back. Kinsman et al (28) later re-enforced the experimental evidence previously available (26) that tent-shaped reliefs (and also more complicated shapes) are indeed produced by monocrystalline ferrite plates. Inasmuch as the PTMC requires that such plates exhibit an invariant plane strain relief effect when formed at a free surface, the finding of tents obviously contradicts the common view that ferrite (and bainite) plates in steel form by shear. More recently, H. J. Lee and Aaronson (29) used TEM to prove that tent-shaped reliefs associated with proeutectoid α plates in a hypoeutectoid Ti-Cr alloy are definitely single crystals.

Bhadeshia (30) reported sometime ago, on the basis of TEM observations, that ferrite plates in an Fe-0.40% C alloy contain a grain boundary along their length, and thus are actually bicrystals. Using the PTMC to analyze selected area electron diffraction determinations of the misorientation of plates in a number of pairs, he concluded that these plates form so that their transformation shears mutually neutralize each other.

It should first be noted that the specimens containing these pairs of plates (which no other investigators have observed either before or since) were isothermally reacted at 700°C and then slowly cooled to room temperature. Particularly given the high reaction rates in high-purity Fe-C alloys, it is probable that the second plate in each pair formed by sympathetic nucleation during cooling below 700°C, rather than isothermally, with the availability of interfacial energy and some degree of supersaturation at the isothermally formed plates having encouraged this process even in the absence of compensating shears (31). The mechanism Bhadeshia proposed for the shear compensation process in an earlier paper requires the presence of a Nishiyama-Wassermann orientation relationship. This relationship does appear in some fcc/bcc transformations (16), but not in steel (32). The crystallography of Bhadeshia's compensation mechanism has also been shown to be incorrect (33).

In the present effort, Bhadeshia's analysis of his orientation relationship data is critically examined. This study was unfortunately made more complicated than necessary because Bhadeshia failed to determine the orientation relationship(s) actually operative in his specimens between the pairs of ferrite plates and their austenite matrix. He merely assumed that the relationship reported by Watson and MacDougall (WM) (34) in their much more thorough investigation of the crystallography of ferrite plates in an Fe-C alloy was applicable to his alloy. Even this relationship, however, is not actually the result of experimental measurements but is rather a compromise between that expected from the PTMC and the WM experimental data on orientation relationships--which themselves displayed considerable scatter. Still further, Bhadeshia's considerations on the crystallography of pairing were incomplete. For cubic crystallography there are 24 variants of a single orientation relationship (OR), resulting in 23 variant combinations. Bhadeshia, however, considered only 8 combinations.

Accordingly, it was necessary during this investigation to consider several different ORs between ferrite and austenite: the Kurdjumow-Sachs, the Nishiyama-Wassermann, the WM and a relationship intermediate between the first two. Matrix algebra was used to manipulate the variants of each of these relationships. These manipulations were based upon the observation of Watson and McDougall (34) that "any two orientations of crystal lattices that are crystallographic variants can be rotated into coincidence by a rigid body rotation that is also a symmetry rotation of the parent lattice". As did Bhadeshia, these rotations can be expressed in terms of "axis/angle pairs", i.e., the axis of rotation of one lattice about the other and the number of degrees through which the rotation was conducted.

The results of this investigation are largely summarized in Tables I - IV and in Fig. 2. In the Tables, attention is called to the directly calculated axis/angle pair and to an equivalent axis/angle pair. When this angle is at or near 180°, cancellation of shears can largely or entirely take place. As shown in the Tables, however, in some cases this angle can be either near 180° or much smaller, and there is no way of distinguishing between the two possibilities.

The overall results of the analyses are summarized stereographically in Fig. 2 on a

$[101]_{bcc}$ stereogram. The range of the axes derived for OR's in the complete range Kurdjumow-Sachs to Nishiyama-Wassermann is shown in this Figure. Note that the variant combinations 1, 5 and 6 lie on the edge of the stereogram and that 7, 8, 11, 13 and 15 are close to symmetry planes. The WD axes can be seen to be very close to one of the variants of Kurdjumow-Sachs. The rotation angles associated with each axis are noted on the diagram, together with Bhadeshia's experimental measurements. In general, the most common pairs studied by Bhadeshia are best described by a rotation of only 1°-2°. This is consistent with a sympathetic nucleation mechanism of forming the second plate, rather than with a shear minimization mechanism.

Bhadeshia, and Wayman and coworkers earlier (35,36) for shape memory martensites, used a simple average of the shape deformation matrices of the variants involved to express quantitatively the degree of mutual cancellation of shape deformation. Wayman et al averaged the shape deformation matrices of four variants and found that they cancel very effectively; the resultant transformation approximates to zero strain to two decimal places at worst and usually to four. No examples were found in the martensite literature examined of two variants mutually cancelling either other's shape deformation.

Bhadeshia's calculations of the cancellation parameter, Ψ, could not be reproduced; instead, much smaller values of Ψ were found. Whereas Wayman et al found that, in shape memory martensites formed in alloys such as Ti-Ni, Ag-Cd, Ni-Al and several Cu-base alloys, Ψ ranged from a maximum of 0.010670 down to 0.000029, Hall's present calculations yielded values from 0.039838 down to 0.00751. This suggests that shape strain cancellation is not a major factor in the formation of the bicrystalline ferrite plates Bhadeshia studied. This should no longer be a surprising result. Wakasa and Wayman (37) have found that packets of parallel martensite laths contain identically oriented crystals of martensite. Similarly, Sandvik (38) has shown that each thin plate of ferrite comprising a sheaf of parallel plates in lower bainite has essentially the same orientation. We are now considering how the failure of this quite reasonable idea might be explained in terms of the invariant line concept.

The results of these considerations will shortly be submitted to Scripta Metallurgica as a discussion to this Bhadeshia (30) paper.

4. ORGANIZATION OF A PACIFIC RIM COUNTRIES CONFERENCE ON THE ROLES OF SHEAR AND DIFFUSION IN THE FORMATION OF PLATES IN CRYSTALLINE SOLIDS

In recent years, and particularly during the present two-year term of this grant, emphasis has been placed upon distinguishing between the roles of diffusion and of shear in the formation of precipitate plates. We have also been much concerned with understanding why the PTMC has often been successfully applied to describe the crystallography and surface relief effect of plates formed during phase transformations which, on the rules enunciated by Christian (25) and Wayman (39), cannot possibly have taken place by a shear mechanism. International interest in these problems has grown greatly in recent years--even though this problem was already active when the classic Davenport and Bain (40,41) paper on the TTT-diagram was presented in 1930. Much of this interest has centered in the so-called Pacific Rim countries: Japan, China, Canada and the United States. In collaboration with Prof. C. Marvin Wayman of the University of Illinois at Urbana-Champaign, with the recently given formal consent of the ASM Phase Transformations Committee, and aided by Prof. John P. Hirth (Washington State Univ.) and Dr. Bhakta B. Rath (Naval Research Laboratory), the P.I. has been working on the programming of a topical conference to be devoted to a serious attempt to resolve the shear vs. diffusional growth issue.

This conference will take place at the Kona-Hilton Hotel, Kona, Hawaii, from December 19 through December 23, 1992. All papers will be invited. All will have equal time. There will be no parallel sessions and no poster sessions. A Panel Discussion (to be chaired by Prof. Hirth) will conclude the Conference. Papers are expected to be prepared by the participants based upon their presentations; these will be submitted to Metallurgical Transactions A for review; all those accepted will be published within one, or at most within two successive issues of Met. Trans. A. Much emphasis will be placed upon both public and private discussions during this conference, and upon inducing the conferees to publish such discussions as are worth preserving. A summary of the Panel Discussion should also be published.

The crux of this conference has been agreed to be the <u>atomic</u> mechanism of the phase transformations to be discussed. Past considerations of this type have too often stopped at showing that a particular transformation obeys some of the requirements of the PTMC, and upon this basis has been declared to be a shear transformation. However, the shearist community is finally beginning to recognize that this is a necessary but not a sufficient proof for identification of the mechanism of a phase transformation as shear. Further, as Wayman (39) has emphasized, in order that a transformation may be so classified it is necessary that all of the requirements of the PTMC be simultaneously obeyed, and that such obedience must occur in a self-consistent manner. Hence, we shall do our best to make clear to the authors that: (i) they must consider all requirements rather than just the one or two with which their experiments or calculations may have dealt; (ii) they must not stop at fulfillment of the formal crystallographic requirements of the PTMC but must move onwards to examine the atomic mechanism; and (iii) they must not ignore relevant research by persons holding the opposed point of view.

By holding this conference in a semi-isolated hotel, by doing our best to hold down attendance to the 50-75 range, by inviting all principal "players" from the Pacific Rim countries (plus selected ones from Europe), and by making every effort, both overt and covert, to promote both public and private discussion, we hope that this conference can make a significant controbution toward resolving that part of this controversy for which enough theory and experimentation already exists, and toward delineating the theoretical analyses and the critical experiments needed to complete the task.

5. MASSIVE TRANSFORMATION IN A Ag-25 A/O Al ALLOY

5.1 Introduction

This is the Ph.D. thesis research of Mr. Yiwen Mou. Its objectives are to ascertain whether or not massive:matrix boundaries are partially coherent, as we predicted that they should be more than 20 years ago from elementary considerations of nucleation theory (42), and to correlate the growth kinetics reported by Perepezko and Massalski (43) in an alloy with nearly the same composition with those predicted by the experimentally observed interfacial structure. TEM is the principal experimental tool being employed in this investigation.

Following Mr. Mou's Ph.D. thesis Overview, in which Professors T. B. Massalski and W. W. Mullins participated, we concluded that unequivocal proof that massive:matrix boundaries really are partially coherent will require that we domonstrate this point with two-dimensional atomic resolution TEM. An instrument suitable for this purpose, a JEOL 4000FX, was being set up in this Department at the time of Mr. Mou's Overview. However, many months elapsed before faults in the instrument (some of which were introduced during installation) could be corrected. This microscope is now operational. However, it does not possess an efficient facility for chilling a thin foil being studied. In consequence, the $\beta \rightarrow \mu_m$ massive transforamtion has been taking place at β:ζ_m boundaries and obscuring them while the foils are being examined. We have managed to improve this situation somewhat by utilizing to the maximum the cold traps in the system; however, problems with μ_m phase formation remain and are continuing to slow the pace of this research. We consider, though, that we will be able to secure sufficient information with two-dimensional atomic resolution and conventional TEM (the latter with a Philips EM420, which does have a liquid nitrogen cold trap) by the expiration of the present grant on Sept. 30, 1991 to complete successfully this program.

5.2 Orientation Relationships

The orientation relationships between ζ_m crystals and their β matrix grains were determined by analyzing diffraction patterns and Kikuchi lines. In addition to the Burgers orientation relationship reported last year, the Potter (44) orientation relationship was found to be operative in the $\beta \rightarrow \zeta_m$ massive transformation. Fig. 3a shows a massive ζ_m crystal in the retained β matrix of a Ag-26 at % Al alloy. The orientation relationship the ζ_m and β phases was determined to be Potter relationship:

$$(1\bar{1}01)_{\zeta_m} // (1\bar{1}0)_\beta$$

$$[11\bar{2}0]_{\zeta_m} // [111]_\beta$$

as demonstrated in the selected area diffraction pattern in Fig. 3b.

5.3 Massive:Matrix Interfacial Structure

More evidence has been accumulated to support the Aaronson-Laird-Kinsman view (2) that massive:matrix interphase boundaries are partially coherent. These include partially coherent structures observed with TEM at Potter-related, Burgers-related, and irrationally oriented interfaces.

5.3.1 Potter Related Interfaces

An example of massive:matrix interfaces where an exact Potter orientation relationship is operative is provided by several planar facets, labeled as A, B, C, D and E in Fig. 4. Fig. 4a is an enlarged image of Fig. 1, and Fig. 4b shows a weak-beam dark-field image clarifying some of the details. Facets B, C and D all contain one set of ledges, but with different directions and slightly different interledge spacings, ranging from 3 to 5 nm. Some irregularly spaced ledges can be seen at facet A. One set of significantly curved ledges dominates facet E, though a second set of irregularly spaced ledges is found in the area close to facet D.

Table V summarizes the contrast behavior of these ledges, as analyzed in Fig. 5, which indicates that they have a Burgers vector of $1/3[\bar{2}113]_{\zeta_m}$. The habit planes of different segments were determined as shown in the stereographic projection in Fig. 6. The habit planes of facets B and C are close to $(\bar{1}101)_{\zeta_m}$, the conjugate plane in the Potter orientation relationship, and lie between $(\bar{1}101)_{\zeta_m}$ and $(0001)_{\zeta_m}$. The habit plane of facet D is also close to $(\bar{1}101)_{\zeta_m}$, but lies between $(\bar{1}101)_{\zeta_m}$ and $(\bar{1}100)_{\zeta_m}$. The habit planes of facets A and E, especially the latter, are far away from $(\bar{1}101)_{\zeta_m}$. In almost all cases, with facet E as a possible exception, the Burgers vector of these ledges is within the terrace plane, $(\bar{1}101)_{\zeta_m}$. In the cases of facets B, C and D, therefore, the uniformly spaced ledges can compensate misfit across the interface; hence they are misfit-compensating ledges, as previously identified by Furuhara et al (11) at the broad faces of α plates in a Ti-Cr alloy.

5.3.2 Burgers-Related Interfaces

Fig. 7 shows a Burgers-related interface between a ζ_m crystal and its retained β matrix. A Burgers orientation relationship, i.e., $(0001)_{\zeta_m}//(0\bar{1}1)_\beta$, $(10\bar{1}0)_{\zeta_m}//(2\bar{1}\bar{1})_\beta$ and $[1\bar{2}10]_{\zeta_m}//[111]_\beta$, was demonstrated by means of the electron diffraction pattern in Fig. 8. Ledge structures were observed on the interface. One set of uniformly spaced and slightly curved ledges has its contrast behavior analyzed in Fig. 9 and Table VI. As a result, the effective Burgers vector associated with this set of ledges is found to be c[0001]. The habit plane was determined to be close to $(\bar{1}010)_{\zeta_m}$, the conjugate plane for the Burgers orientation relationship. The direction of these c-type ledges was found to be perpendicular to their effective Burgers vector. The interledge spacing for these ledges is about 14 nm.

The ledge direction and the apparent habit plane determined by trace analysis of the Burgers-related interface are shown in the $[0001]_{\zeta_m}$ stereographic projection in Fig. 10. In this figure are also shown the ledge direction and apparent habit plane of the near-Burgers-related interface reported last year. (This interface was termed Burger-related, but it actually had a very small deviation, less than 2°, from the exact Burgers orientation relationship.) The effective

Burgers vectors in these two cases are presented in the stereographic projection. The same conjugate planes, i.e., $(\bar{1}010)_{\zeta_m}//(\bar{2}11)_{\beta}$, can be expected for them. The apparent habit planes, however, turn away from the conjugate plane in different directions. As a result, different effective Burgers vectors and ledge directions are obtained.

Very fine linear defects, about 3 nm apart, are present on this Burgers-related interface, as shown in Figs. 7 and Fig. 9d. These two images were taken with different $\underline{g}$ vectors, i.e., $(0002)_{\zeta_m}$ for Fig. 7 and $(01\bar{1}1)_{\zeta_m}$ for Fig. 9d. Therefore, these fine lines are not Moire fringes. Since their spacing is the same in these Figures they are probably also ledges of very small height. In the presence of c-type ledges approximately along the $[1\bar{2}10]_{\zeta_m}$ direction, the apparent habit plane can only deviate from $(\bar{1}010)_{\zeta_m}$ toward $(0001)_{\zeta_m}$. The presence of these very fine ledges approximately along the $[0001]_{\zeta_m}$ direction can help to explain the deviation from the $(\bar{1}101)_{\zeta_m}$ toward the $(1\bar{2}10)_{\zeta_m}$ apparent habit plane. However, these very fine ledges may also be of the misfit-compensating type.

Growth ledges are demonstrated very clearly on this Burgers-related interface (Fig. 7). From the huge deflections of the uniformly spaced ledges the growth ledges induce, the height of these growth ledges was estimated to be 25 nm.

5.3.3 Irrationally-Related Interfaces

Ledge structures were also observed on massive:matrix interfaces across which the massive crystals and the β matrix grains are irrationally oriented. Fig. 11 shows an example of this situation. The orientation relationship of this ζ_m crystal with respect to its β grain deviates greatly from the Burgers orientation relationship, as described in the $[0001]_{\zeta_m}$ stereographic triangle in Fig. 12. The close-packed planes in the two phases are rotated 27° apart, and the close-packed directions are 57° apart.

As shown in Fig. 11 this interface does not appear to be particularly flat, probably because it contains many irregular line defects. The lines in the left hand portion of the interface are much closer to one another than those in the right hand portion. These lines are thought to be growth ledges. Fig. 13 indicates another segment in the same interface as that of Fig. 11, with a rotation about 75° from the boundary direction in Fig. 11. In the left end of this segment only growth ledges can be seen. In the middle portion, however, regularly arranged and uniformly spaced ledges are present. The interledges spacing is about 5 nm.

When an irrational orientation relationship is associated with massive crystals and their matrix grains, atomic matching across interphase boundaries is unlikely to be as good as it is across rationally-oriented interfaces. Consequently, ledges or misfit dislocations in this case would be much more closely spaced. Such densely distributed ledges or dislocations may be difficult to observe, however, due to the resolution limitation of the Philips 420 microscope. In a few cases, however, when the orientation relationship and boundary orientation are combined to favor better atomic matching, the misfit-compensating defects will be resolved. The middle portion of the interface in Fig. 13 shows a twist rotation relative to both the left and right portions; this may be responsible for resolution of the ledge structure in this area of the interface.

5.4 Graphical and O-Lattice Modeling of Interfacial Structures

The graphical technique first employed by Rigsbee and Aaronson (45) and recently by Furuhara and Aaronson (46) was used to analyze the partial coherent structures of the massive:matrix boundaries. The lattice parameters chosen were a_β = 0.324 nm, a_{ζ_m} = 0.2865 nm and c_{ζ_m} = 0.4653 nm (5); these were determined for a Ag-25.8 at % Al alloy reacted in the temperature range 605° to 700°C. These conditions are almost identical to those in the present research. Bollmann (47) O-lattice calculations were also made for the massive:matrix interphase boundaries with the same lattice parameters.

Fig. 14 shows the structure of the $(1\bar{1}00)_{\zeta_m}//(\overline{2}\bar{1}\bar{1})_\beta$ interface, across which a Burgers orientation relationship is assumed, obtained with the graphical technique. The coherent patches, defined by pairs of atomic positions in the two phases with a spacing less than 15% of the average close packed distance between them, form a rectangular pattern. In order to compensate misfit across this interface so as to form a partially coherent boundary, two sets of misfit-compensating defects are needed in orthogonal directions. Fig. 15 shows results from the O-lattice calculation, which are almost identical to those in Fig. 14. Two sets of misfit-compensating defects lie in $[0001]_{\zeta_m}$ and $[11\bar{2}0]_{\zeta_m}$ directions, with their Burgers vectors being $\underline{a}[11\bar{2}0]_{\zeta_m}$ and $\underline{c}[0001]_{\zeta_m}$, and inter-defect spacings 30.1 nm and 13.6 nm, respectively.

The TEM observations shown in Fig. 7 now can be compared with the modeling results. One set of misfit-compensating ledges with Burgers vector $\underline{c}[0001]$ lying approximately in the $[11\bar{2}0]_{\zeta_m}$ direction can obviously serve as the horizontal line defects in Fig. 15. With an actual spacing being about 14 nm, the effective Burgers vector associated with these misfit-compensating ledges is probably $\underline{c}/2[0001]$ as was found in a Ti-Cr alloy (17). There is also another set of line defects at the interface in Fig. 7, lying perpendicular to the first set. Although its Burgers vector was not determined because of its very weak contrast, this set probably compensates misfit in the $[11\bar{2}0]_{\zeta_m}$ direction.

Figs 16 and 17 are partially coherent structures of the $(0001)_{\zeta_m}//(0\bar{1}1)_\beta$ interface, with a Burgers orientation relationship again assumed, obtained by the graphical technique and O-lattice calcuation, respectively. Since the coherent patches or O-points are much more densely distributed than at the $(1\bar{1}00)_{\zeta_m}//(2\bar{1}\bar{1})_\beta$ interface, many more misfit-compensating defects per unit area will be necessary. As a result, this type of massive:matrix interface will have much higher interfacial energy. No conjugate plates of this type have so far been observed at a Burgers orientation relationship.

The partially coherent interface associated with the Potter orientation relationship was also modeled; the results are presented in Fig. 18 from the graohical technique and in Fig. 19 from the O-lattice calcuation. Two sets of misfit-compensating defects intersect at an angle of 17.5°. The more densely spaced set has an inter-defect spacing of 4.1 nm and a Burgers vector of $1/3[\bar{2}113]_{\zeta_m}$. Such defects are probably misfit compensating ledges. These defects were observed with TEM, as shown in Fig. 4. It is easy to understand that the other set only can be occasionally observed because its spacing is predicted to be more than 100 nm, the same order of magnitude as the width of an interface observed in TEM specimens.

6. FUTURE PLANS

6.1 Generic Overviews and Other Papers

The invited paper assessing comparisons between homogeneous nucleation theory and experiment will first be completed. Then the overview of ledgewise growth in vapor → crystal, liquid → crystal and crystal → crystal phase transformations will be completed. Our Institute of Metals lecture paper "On the Atomic Mechanisms of Diffusional Nucleation and Growth" will be written next. This will be followed by a concise overview of the diffusionist viewpoint on the bainite reaction for the Materials Transactions of the JIM special issue on the bainite reaction. The remainder of this grant year will be devoted to writing or completing papers based upon research performed with the support of this and our now completed NSF grant (for nucleation and interfacial energy research).

6.2 Collaborative Research with Dr. M. G. Hall

Writing of the Discussion to a paper by Bhadeshia (30) will first be completed. A literature search is then planned by Dr. Hall on differences between the habit planes of plates formed diffusionally and those produced by a martensitic mechanism. An effort will then be made to rationalize these differences in terms of differences in the orientation of the Burgers vector of the misfit-compensating defects/LID dislocations on the terraces of the ledges on the broad faces of these plates. Following writeup of this work, an analysis will be undertaken of the origin of tent-shaped surface relief effects in diffusional transformations proceeding by means of the ledge mechanism.

6.3 Massive Transformation in Ag-26 A/O Al Alloy

Every effort will be made to conduct a two-dimentional atomic resolution TEM study of partially coherent massive:matrix interfaces. Particular efforts will be devoted to imaging and then analyzing, both graphically and via the O-lattice analysis (47), the nature, geometry and distribution of misfit compensating-defects in $\beta:\zeta_m$ interfaces. Time permitting, hot-stage TEM studies will also be made of the kinetics of ledgewise growth of the massive transformation under investigation and the results of these measurements and the interfacial structure studies will be used to explain the growth kinetics data of Perepezko and Massalski (43) on a Ag-Al alloy with nearly the same composition. Mr. Yiwen Mou will then write his Ph.D. thesis and the papers to be derived from it.

REFERENCES

1. M. R. Plichta, J. C. Williams and H. I. Aaronson, Met. Trans., 8A, 1885 (1977).
2. J. W. Gibbs, Collected Works, 1, pp. 105, 252. Yale Univ. Press, New Haven, CT (1948).
3. K. Binder and D. Stauffer, Advances in Phys., 25, 343 (1976).
4. J. S. Langer and A. J. Schwartz, Phys. Rev. A, 21, 948 (1980).
5. I. Servi and D. Turnbull, Acta Met., 14, 161 (1966).
6. D. H. Kirkwood, Acta Met., 18, 563 (1970).
7. A. W. West and D. H. Kirkwood, Scripta Met., 10, 681 (1976).
8. T. Hirata and D. H. Kirkwood, Acta Met., 25, 1425 (1977).
9. F. K. LeGoues and H. I. Aaronson, Acta Met., 32, 1855 (1984).
10. J. W. Cahn and J. E. Hilliard, Jnl. Chem. Phys., 31, 539 (1959).
11. H. E. Cook, D. de Fontaine and J. E. Hilliard, Acta Met., 17, 765 (1969).
12. H. E. Cook and D. de Fontaine, 17, 915 (1969).

13. P. Haasen, Met. Trans., 16A, 1173 (1985).

14. J. W. Christian, Physical Properties of Martensite and Bainite, Iron and Steel Inst., London, p. 129 (1969).

15. H. I. Aaronson, T. Furuhara, J. M. Rigsbee, W. T. Reynolds, Jr. and J. M. Howe, Met. Trans., 21A, 2369 (1990).

16. M. G. Hall, H. I. Aaronson and K. R. Kinsman, Surface Science, 31, 257 (1972).

17. T. Furuhara, J. M. Howe and H. I. Aaronson, submitted to Acta Met.

18. H. I. Aaronson, C. Laird and K. R. Kinsman, Phase Transformations, ASM, Materials Park, OH, p. 313 (1970).

19. U. Dahmen, Scripta Met., 21, 1029 (1987).

20. J. M. Lang, U. Dahmen and K. H. Westmacott, Acta Met., 34, 475 (1986).

21. Z. Nishiyama, Sci. Rep. Tohoku Univ., 23, 638 (1934).

22. G. Wassermann, Arch. Eisenhuttenwesen, 16, 647 (1933).

23. H. I. Aaronson, J. K. Lee and K. C. Russell, Precipitation Processes in Solids, TMS, Warrendale, PA, p. 31 (1978).

24. C. M. Wayman, Advances in Materials Research, 3, 147 (1968).

25. J. W. Christian, Dislocations and Properties of Real Materials, Inst. of Metals, London, p. 94 (1985).

26. H. I. Aaronson, The Mechanism of Phase Transformations in Crystalline Solids, Inst. of Metals, London, p. 270 (1969).

27. G. R. Srinivasan and C. M. Wayman, ibid, p. 310.

28. K. R. Kinsman, E. Eichen and H. I. Aaronson, Met. Trans., 6A, 303 (1975).

29. H. J. Lee and H. I. Aaronson, Acta Met., 36, 787 (1988).

30. H. K. D. H. Bhadeshia, Acta Met., 29, 1117 (1981).

31. H. I. Aaronson and W. T. Reynolds, Jr., Scripta Met., 21, 1599 (1987).

32. H. I. Aaronson, Scripta Met., 14, 825 (1980).

33. U. Dahmen, Scripta Met., 15, 73 (1981).

34. J. D. Watson and P. G. McDougall, Acta Met., 21, 961 (1973).

35. S. Miyazaki and C. M. Wayman, Acta Met., 36, 181 (1988).

36. T. Saburi and C. M. Wayman, Acta Met., 21, 979 (1979).

37. K. Wakasa and C. M. Wayman, Metallography, 14, 49 (1981).

38. B. P. J. Sandvik, Met. Trans., 13A, 777 (1982).

39. H. McI. Clark and C. M. Wayman, Phase Transformations, ASM, Materials Park, OH, p. 59 (1970).

40. E. S. Davenport and E. C. Bain, Trans. AIME, 90, 117 (1930).

41. S. L. Hoyt, discussion to ref. 40.

42. H. I. Aaronson, C. Laird and K. R. Kinsman, Scripta Met., 2, 259 (1968).

43. J. H. Perepezko and T. B. Massalski, Acta Met., 23, 621 (1975).

44. D. I. Potter, Jnl. Less Common Metals, 31, 299 (1973).

45. J. M. Rigsbee and H. I. Aaronson, Acta Met., 27, 351 (1979).

46. T. Furuhara and H. I. Aaronson, submitted to Acta Met.

47. W. Bollmann, Crystal Defects and Crystalline Interfaces, Springer-Verlag, Berlin (1970).

LIST OF FIGURE CAPTIONS

Fig. 1 A geometrically glissile invariant plane strain interface; structural ledges are $11\underline{\mu}$; steps introduced by LID dislocations are $11\underline{v}$. After Dahmen (19).

Fig. 2 $[101]_{bcc}$ stereogram showing the locations of axis/angle pairs calculated for ORs in the range K-S to N-W. The OR derived by Watson and McDougall (34) and experimental data due to Bhadeshia (30) are also included.

Fig. 3 TEM micrographs showing a faceted massive:matrix interface, across which a Potter orientation relationship is operative: (a) bright field micrograph, and (b) selected area diffraction pattern.

Fig. 4 TEM micrograph showing ledge structure on a Potter-related interface: (a) bright field micrograph, and (b) weak-beam dark-field micrograph.

Fig. 5 TEM micrographs of a Potter-related massive:matrix interface, imaged with seven different reflections from the ζ_m phase: (a) $(0002)_{\zeta_m}$, (b) $(11\bar{2}0)_{\zeta_m}$, (c) $(10\bar{1}1)_{\zeta_m}$, (d) $(\bar{1}011)_{\zeta_m}$, (e) $(02\bar{2}0)_{\zeta_m}$, (f) $(01\bar{1}1)_{\zeta_m}$, and (g) $(0\bar{1}11)_{\zeta_m}$.

Fig. 6 A $(11\bar{2}0)_{hcp}$ stereographic projection displaying results from trace and Burgers vector analyses for the Potter-related interface.

Fig. 7 TEM micrograph showing ledge structures on a Burgers-related interface.

Fig. 8 Selected area diffraction pattern showing a Burgers orientation relationship.

Fig. 9 TEM micrographs of a Burgers-related interface, imaged with four different reflections from the ζ_m phase: (a) $(0002)_{\zeta_m}$, (b) $(0\bar{1}11)_{\zeta_m}$, (c) $(11\bar{2}0)_{\zeta_m}$, and (d) $(01\bar{1}1)_{\zeta_m}$.

Fig. 10 A $(0001)_{hcp}$ stereographic projection displaying results from trace and Burgers vector analyses for a near-Burgers-related and Burgers-related massive:matrix interfaces.

Fig. 11 TEM micrograph of an irrationally-related massive:matrix interface.

Fig. 12 A $(0001)_{\zeta_m}$ stereographic triangle showing an irrational orientation relationship between a ζ_m crystal and its β matrix grain.

Fig. 13 TEM micrograph of an irrationally-related massive:matrix interface showing a ledged middle portion.

Fig. 14 Computer plot of coherent patches and misfit dislocation structures on the $(1\bar{1}00)_{\zeta_m}//(2\bar{1}\bar{1})_\beta$ interface.

Fig. 15 Computer plot of O-points and misfit dislocation structures on the $(1\bar{1}00)_{\zeta_m}//(2\bar{1}\bar{1})_\beta$ interface.

Fig. 16 Computer plot of coherent patches and misfit dislocation structures on the $(0001)_{\zeta_m}//(0\bar{1}1)_\beta$ interface.

Fig. 17 Computer plot of O-points and misfit dislocation structures on the $(0001)_{\zeta_m}//(0\bar{1}1)_\beta$ interface.

Fig. 18 Computer plot of coherent patches and misfit dislocation structures on the $(1\bar{1}01)_{\zeta_m}//(1\bar{1}0)_\beta$ interface.

TABLE CAPTIONS

Table I Summary of Axis/Angle Pair Relationships - N-W OR.

Table II Summary of Axis/Angle Pair Relationships - K-S OR.

Table III Summary of Axis/*angle Pair Relationships - $\Theta = 2°$.

Table IV Summary of Axis/Angle Pair Relationships - Watson & McDougall OR.

Table V Observed and Calculated Contrast Behavior for a Potter OR Interface.

Table VI Observed and Calculated Contrast Behavior for a Burgers OR Interface.

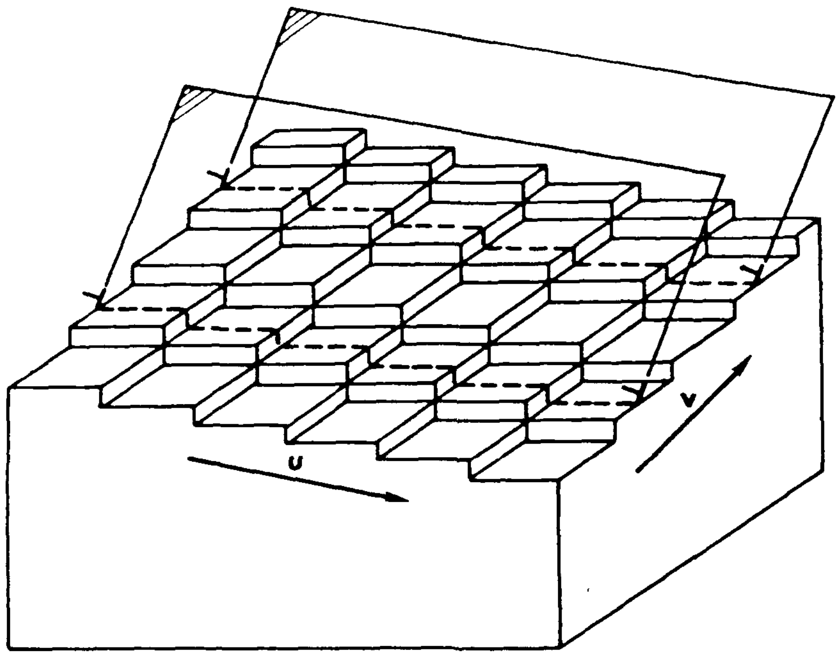


Figure 1

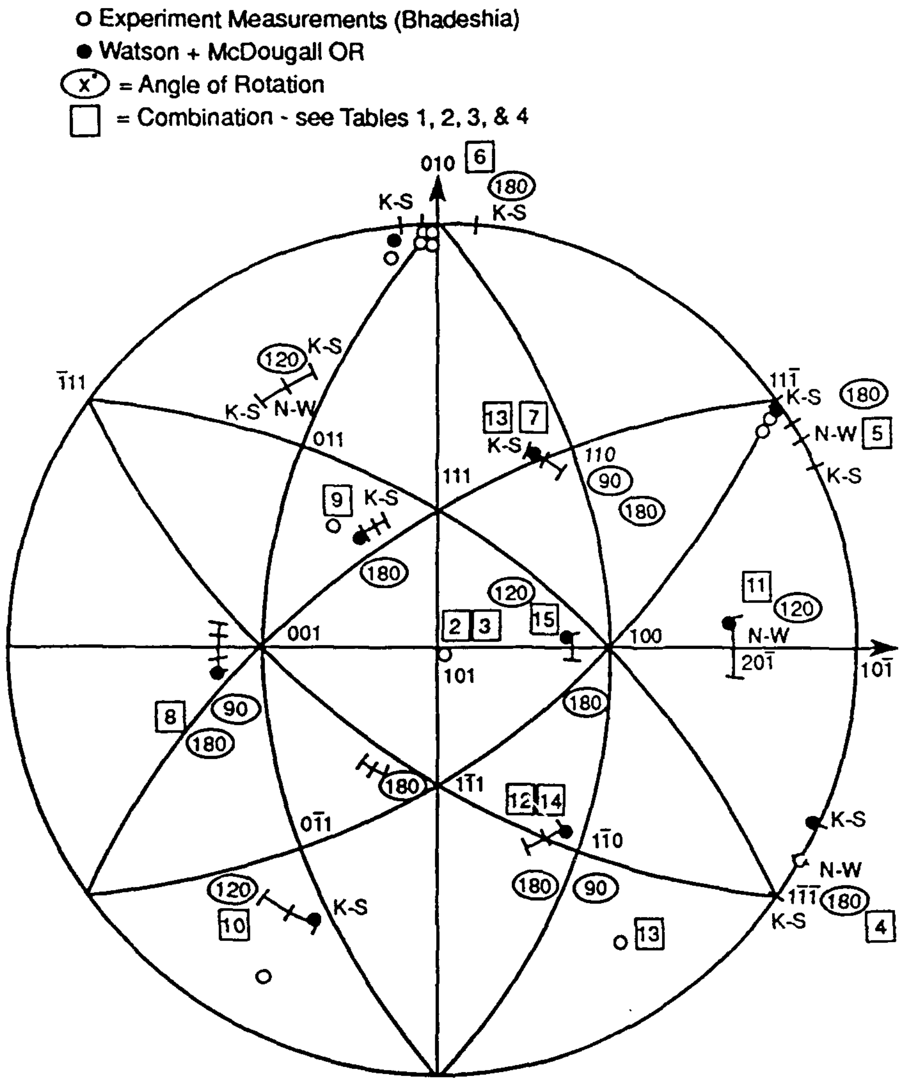
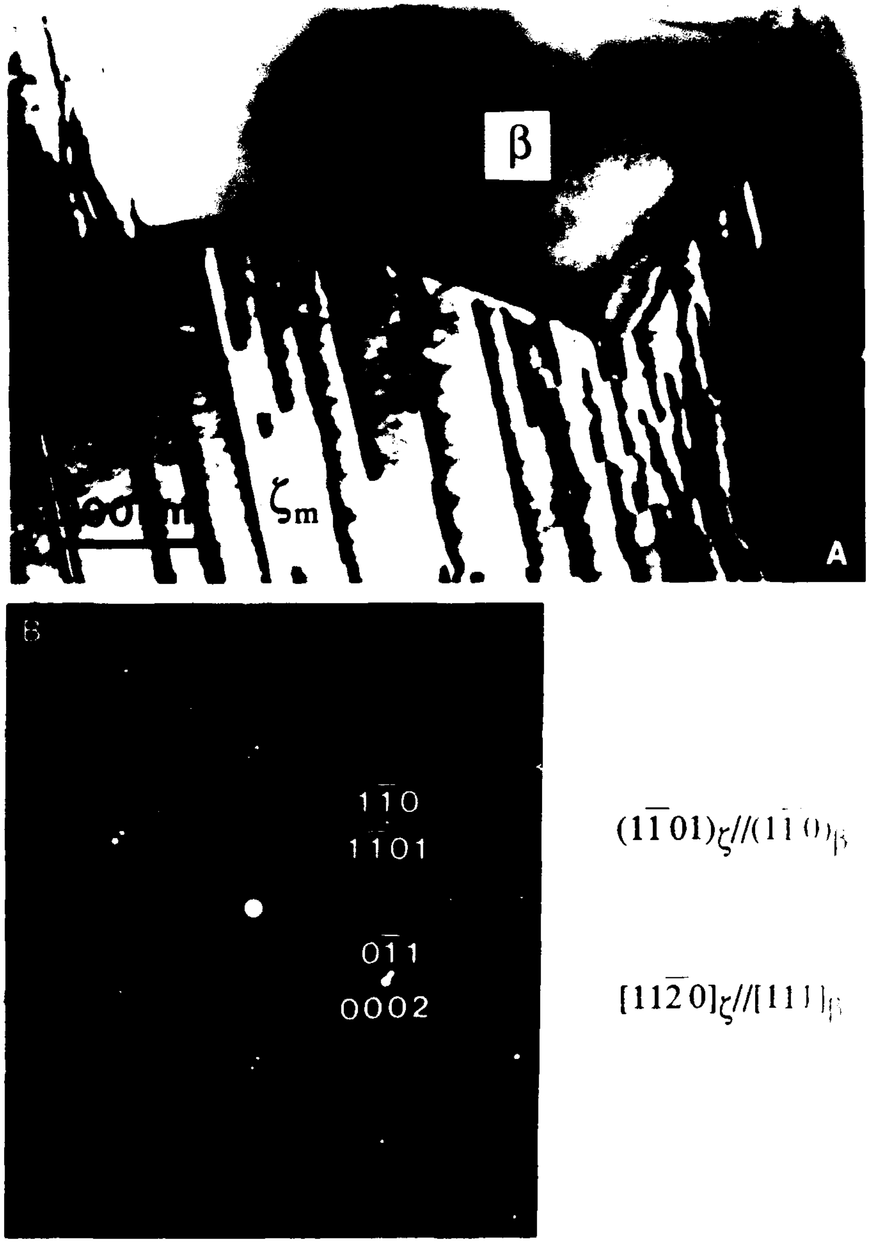

o Experiment Measurements (Bhadeshia)
● Watson + McDougall OR
(x°) = Angle of Rotation
□ = Combination - see Tables 1, 2, 3, & 4
010
6
180
K-S
K-S
120
K-S
K-S
N-W
$\bar{1}11$
011
111
13
7
K-S
110
90
180
$11\bar{1}$
K-S
180
N-W
5
K-S
9
K-S
180
120
11
120
2
3
15
001
101
100
N-W
$20\bar{1}$
$10\bar{1}$
8
90
180
180
180
$1\bar{1}1$
12
14
$0\bar{1}1$
$1\bar{1}0$
K-S
N-W
$1\bar{1}\bar{1}$
180
K-S
4
120
10
K-S
180
90
13

Figure 2



$(1\bar{1}01)_{\zeta} // (1\bar{1}0)_{\beta}$

$[11\bar{2}0]_{\zeta} // [111]_{\beta}$

Figure 3

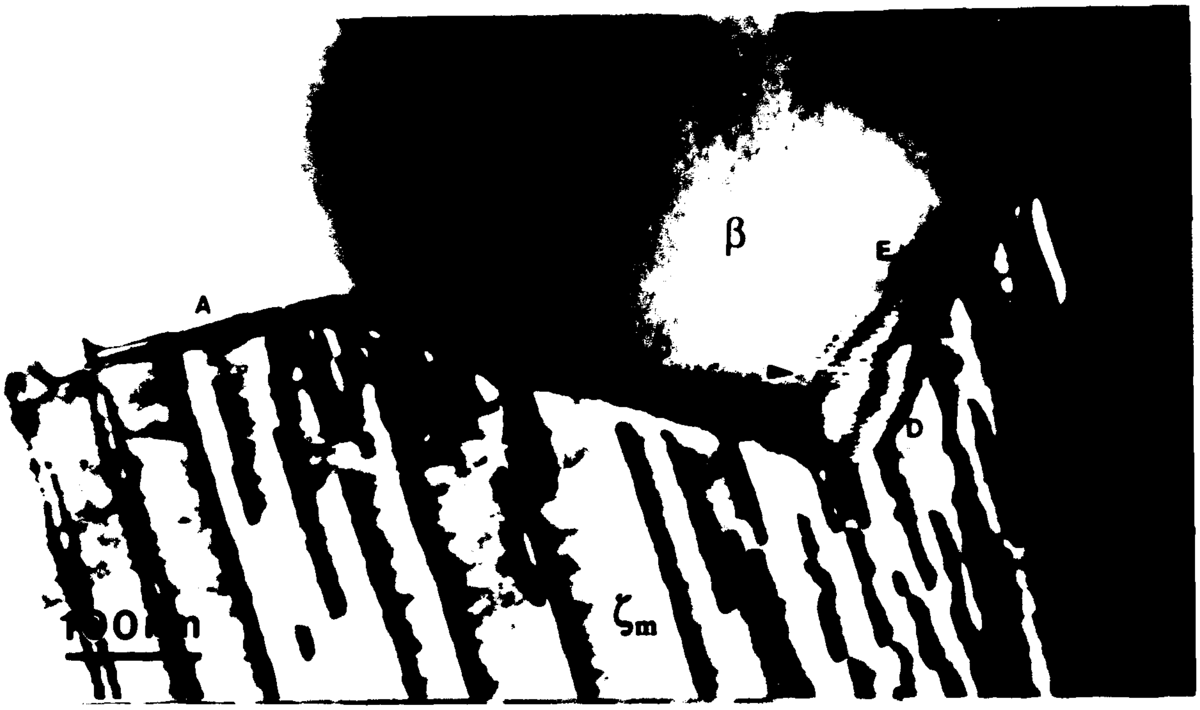


Figure 4

Figure 4
Continued

Figure 5

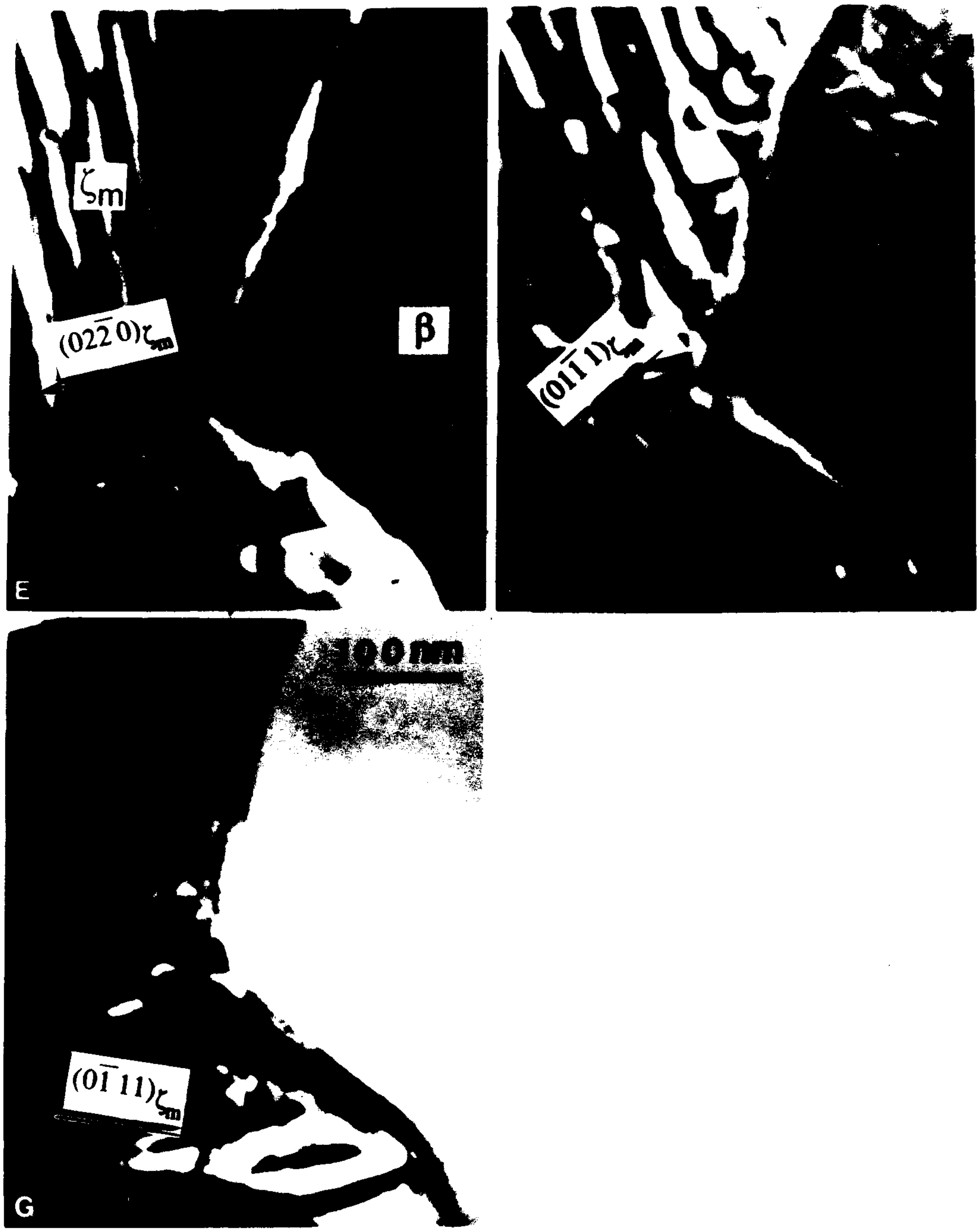


Figure 5
Continued

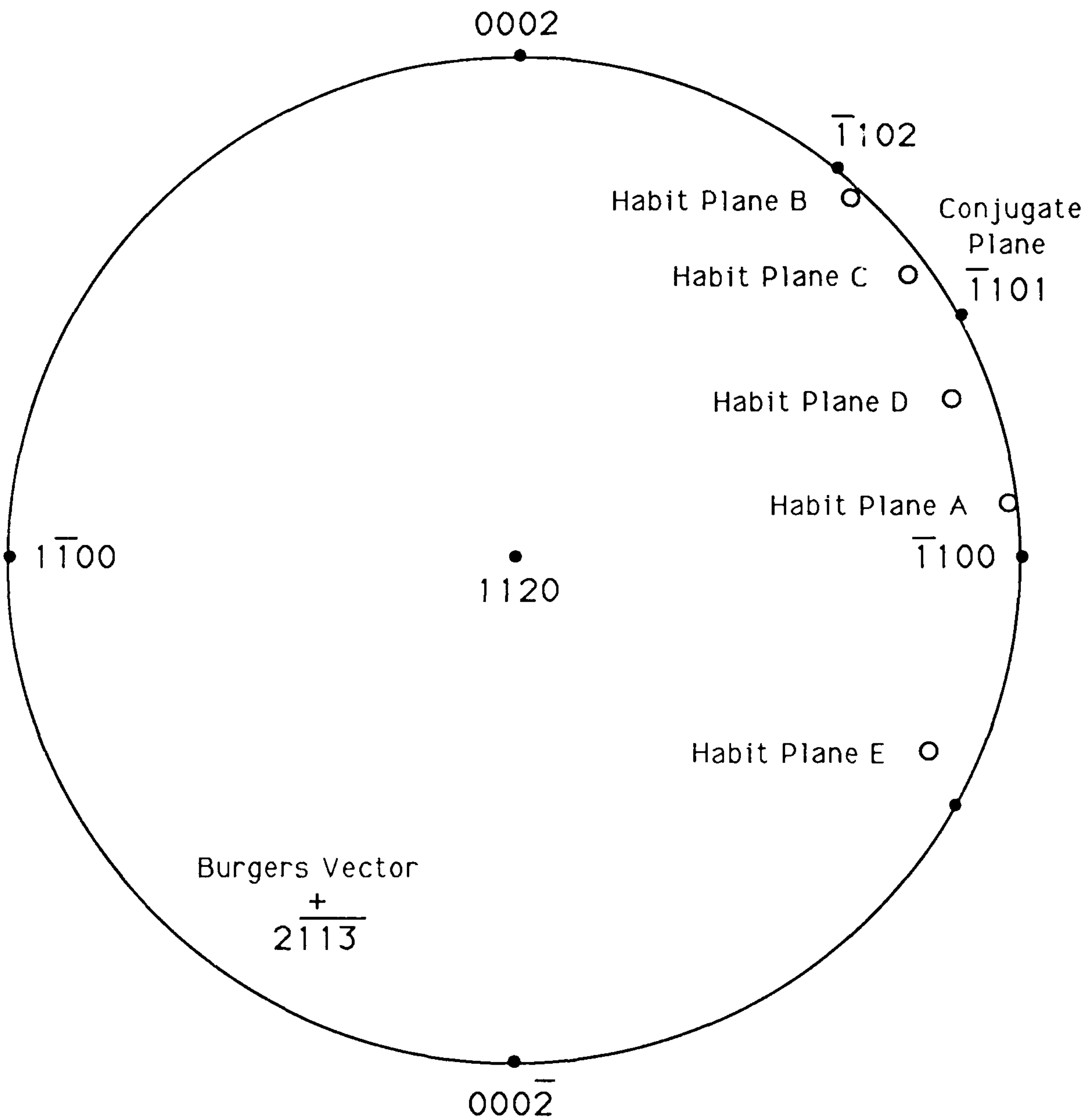

0002
$\bar{1}102$
Habit Plane B
Conjugate Plane
Habit Plane C
$\bar{1}101$
Habit Plane D
Habit Plane A
$1\bar{1}00$
$\bar{1}100$
1120
Habit Plane E
Burgers Vector
+
$\overline{2113}$
$000\bar{2}$

Figure 6

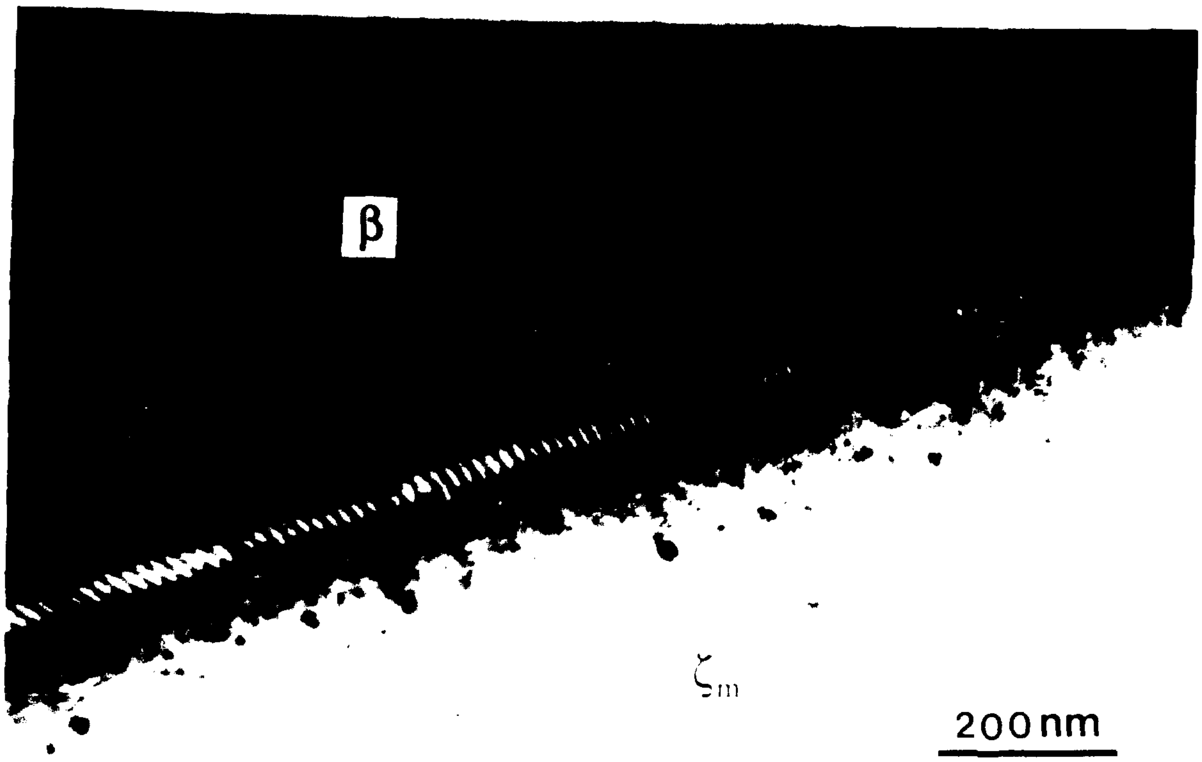
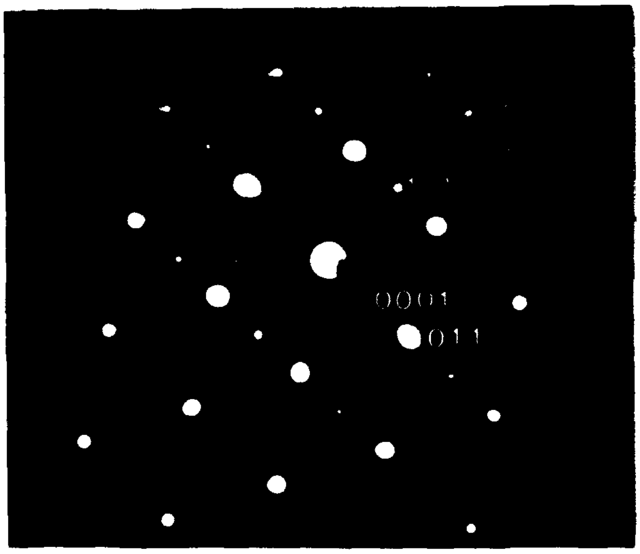


Figure 7



$(0001)_\zeta // (0\bar{1}1)_\beta$

$[\bar{1}100]_\zeta // [\bar{2}11]_\beta$

$[11\bar{2}0]_\zeta // [111]_\beta$

Figure 8

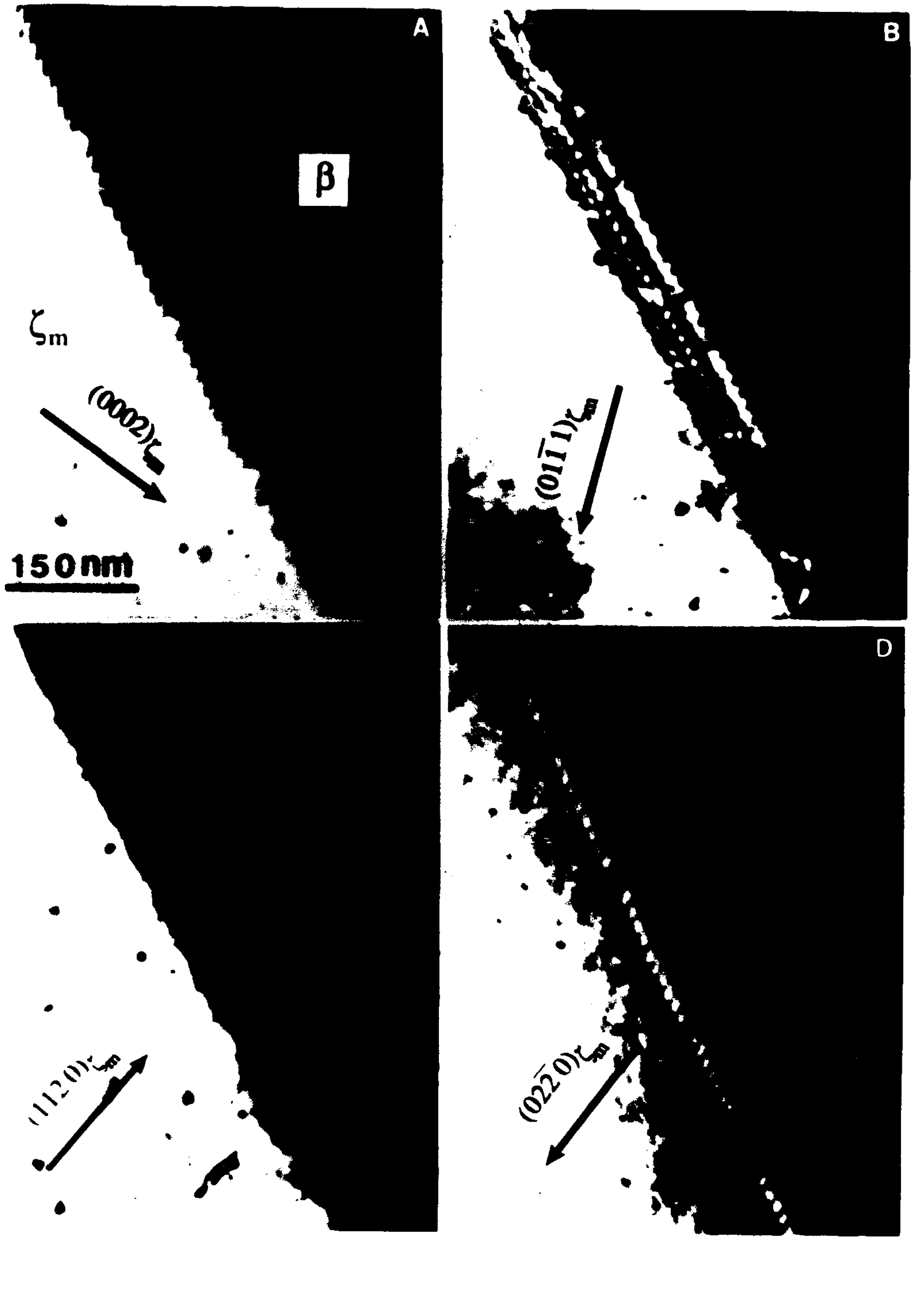
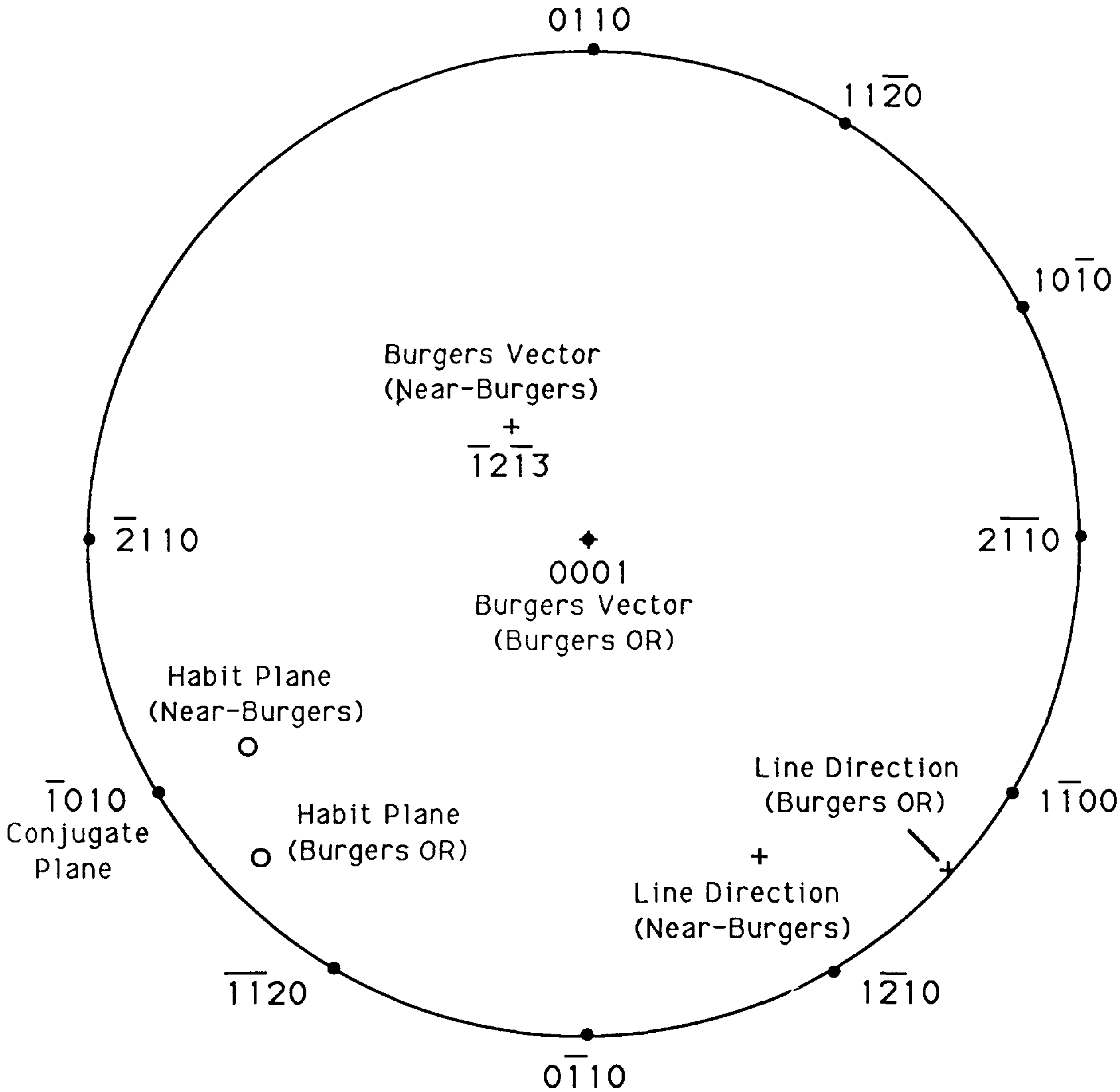

A
β
ζ_m
$(0002)_{\zeta_m}$
150nm
B
$(01\bar{1}1)_{\zeta_m}$
$(11\bar{2}0)_{\zeta_m}$
D
$(02\bar{2}0)_{\zeta_m}$

Figure 9



0110
11$\bar{2}$0
10$\bar{1}$0
Burgers Vector
(Near-Burgers)
$\bar{1}$2$\bar{1}$3
$\bar{2}$110
2$\bar{1}\bar{1}$0
0001
Burgers Vector
(Burgers OR)
Habit Plane
(Near-Burgers)
Line Direction
(Burgers OR)
$\bar{1}$010
Conjugate
Plane
Habit Plane
(Burgers OR)
1$\bar{1}$00
Line Direction
(Near-Burgers)
$\bar{1}\bar{1}$20
1$\bar{2}$10
0$\bar{1}$10

Figure 10

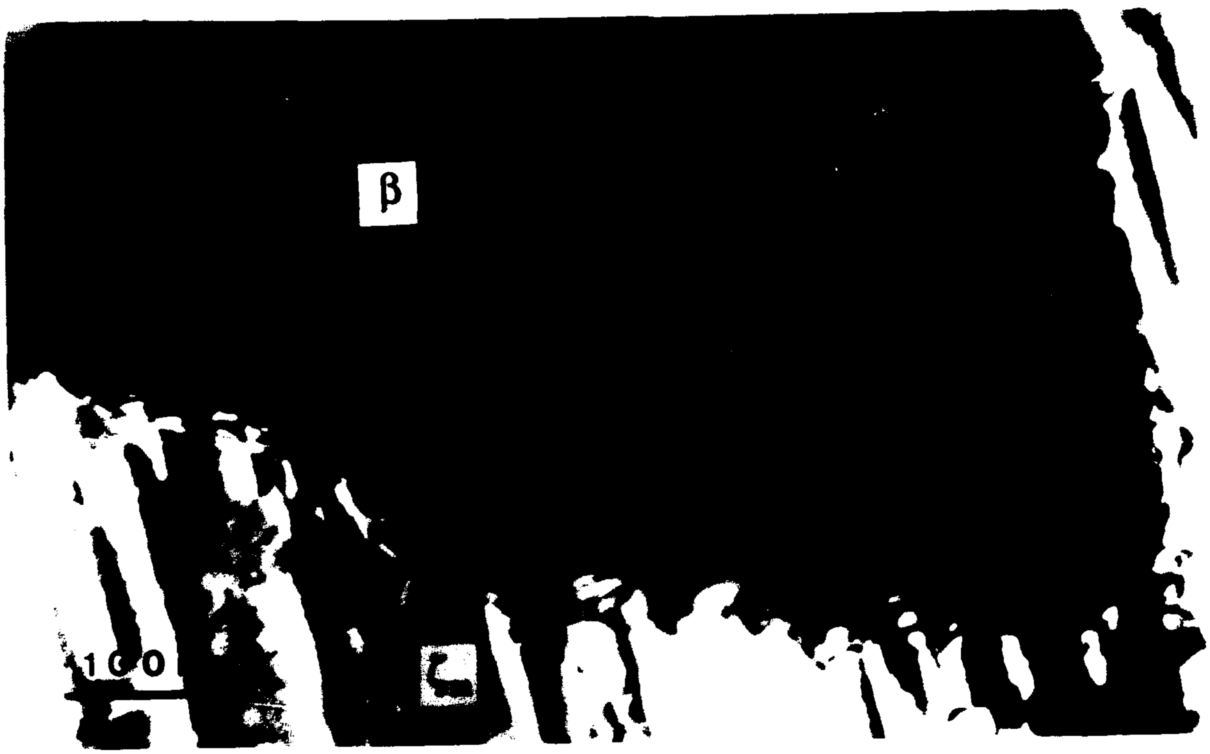
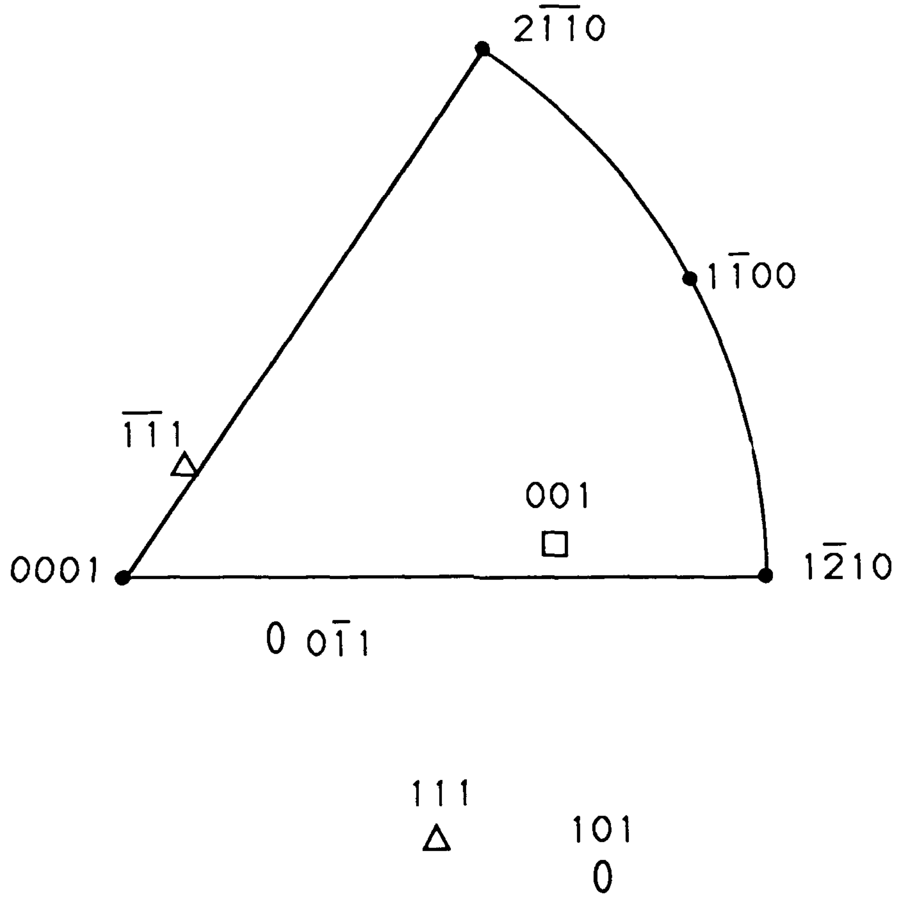


Figure 11



$2\bar{1}\bar{1}0$
$1\bar{1}00$
$\bar{1}\bar{1}1$
001
0001
$1\bar{2}10$
$0\ 0\bar{1}1$
111
101
0

Figure 12

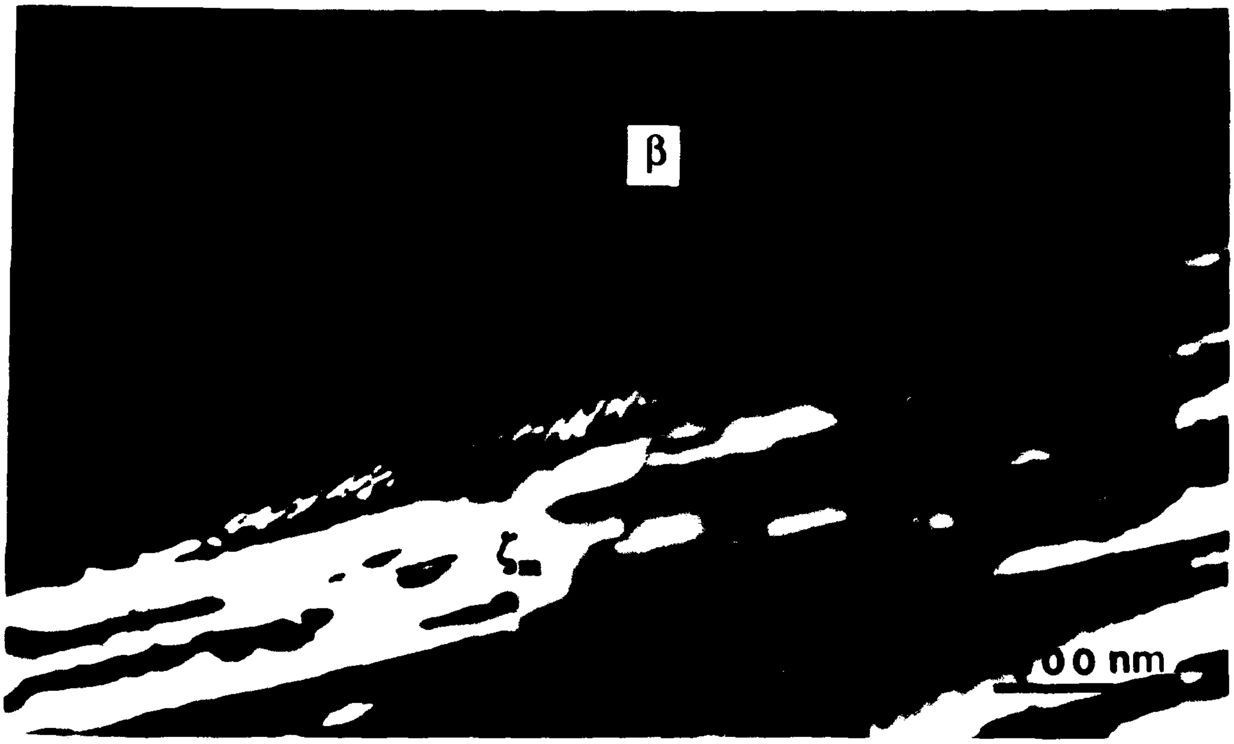


Figure 13

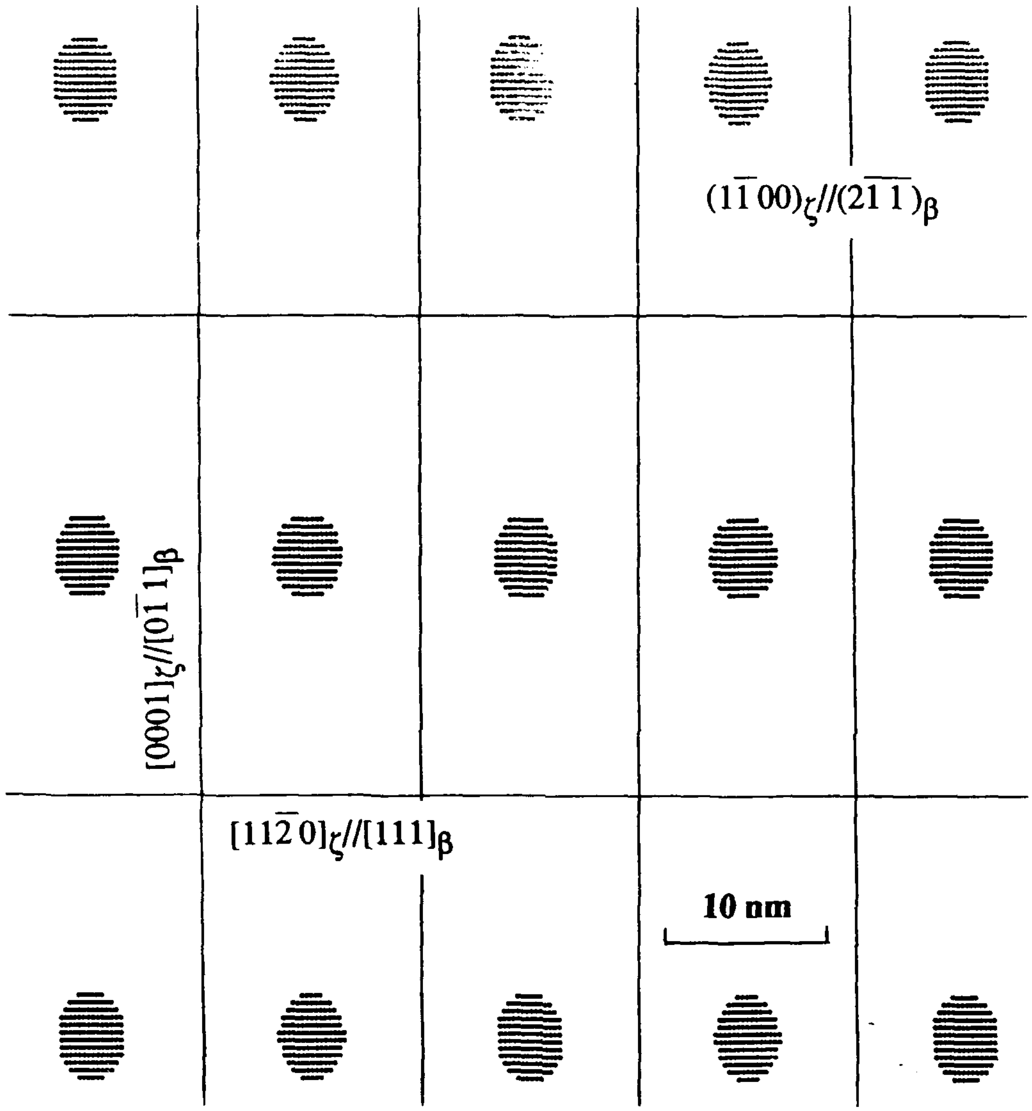

$(1\bar{1}00)_\zeta//(2\bar{1}\bar{1})_\beta$
$[0001]_\zeta//[0\bar{1}1]_\beta$
$[11\bar{2}0]_\zeta//[111]_\beta$
10 nm

Figure 14

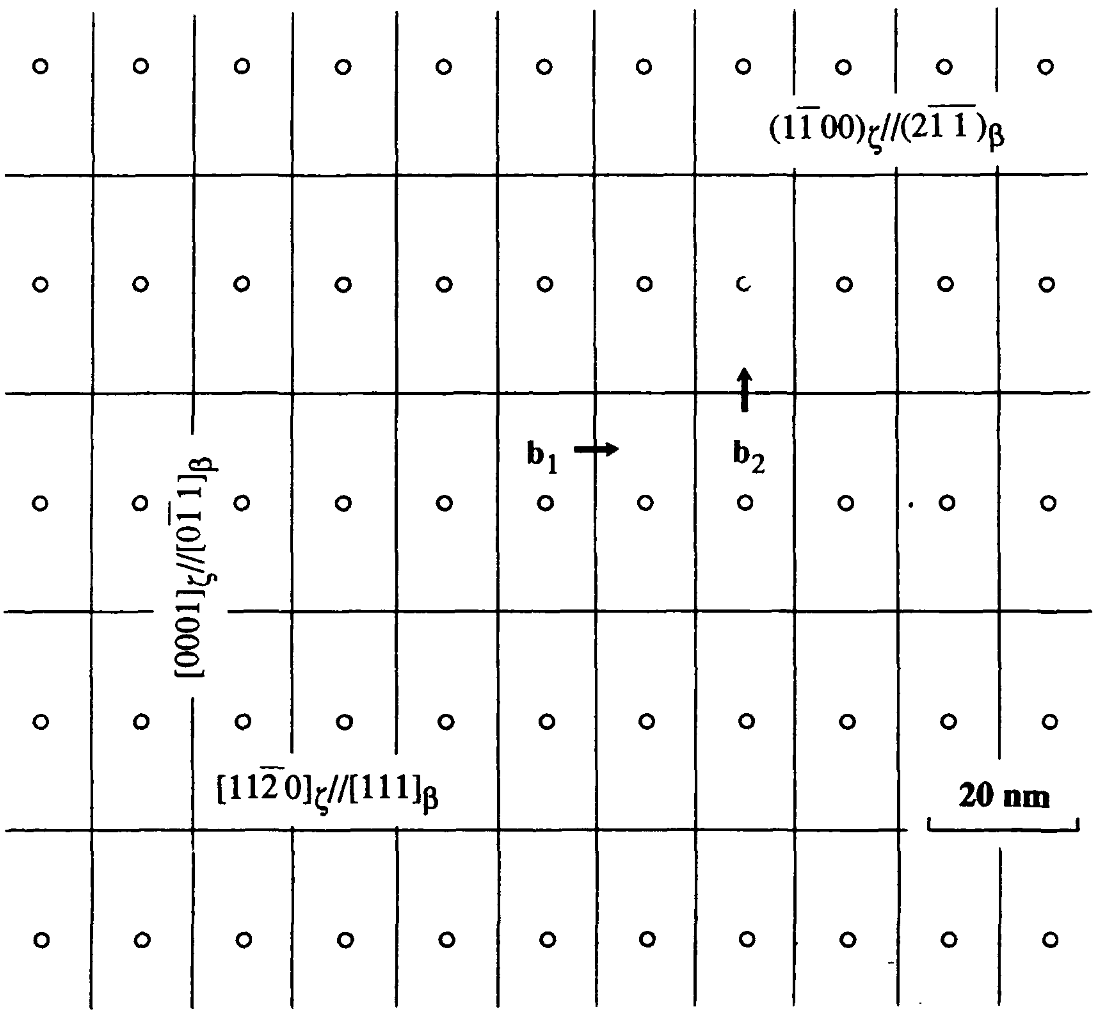

$(1\bar{1}00)_\zeta//(2\bar{1}\bar{1})_\beta$
$\mathbf{b}_1$
$\mathbf{b}_2$
$[0001]_\zeta//[0\bar{1}1]_\beta$
$[11\bar{2}0]_\zeta//[111]_\beta$
20 nm

Figure 15

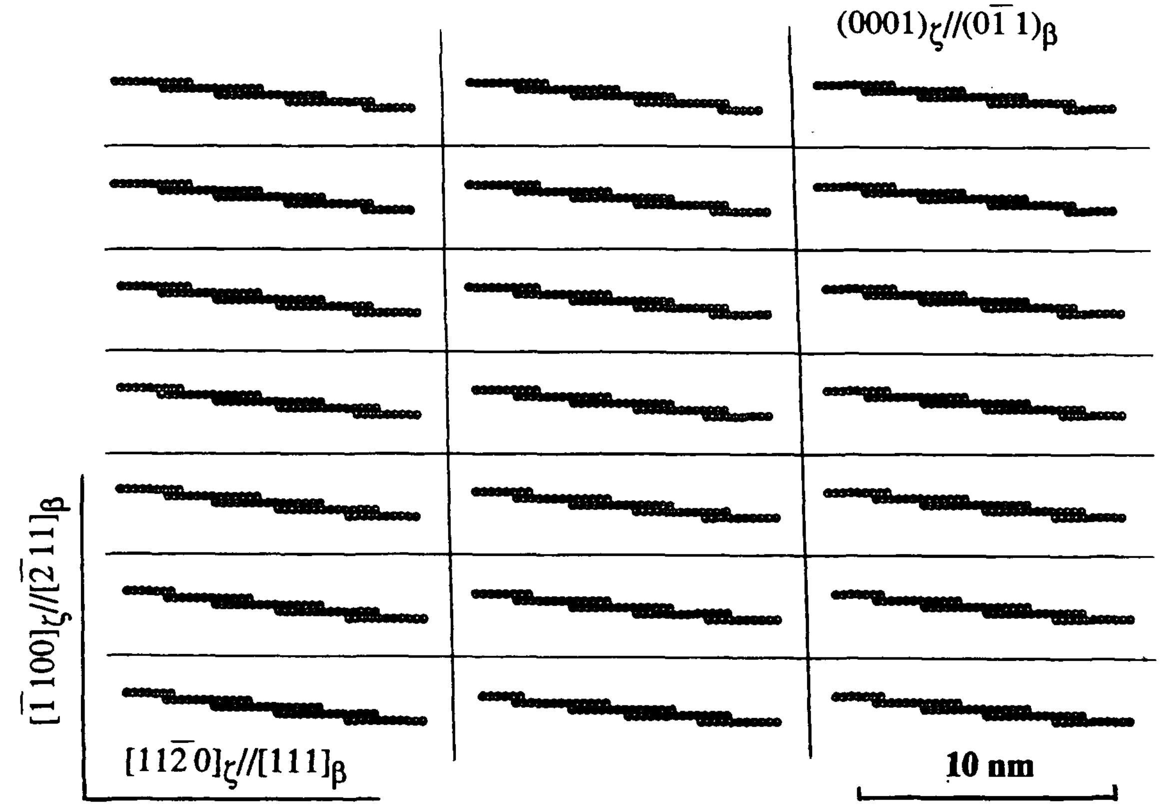
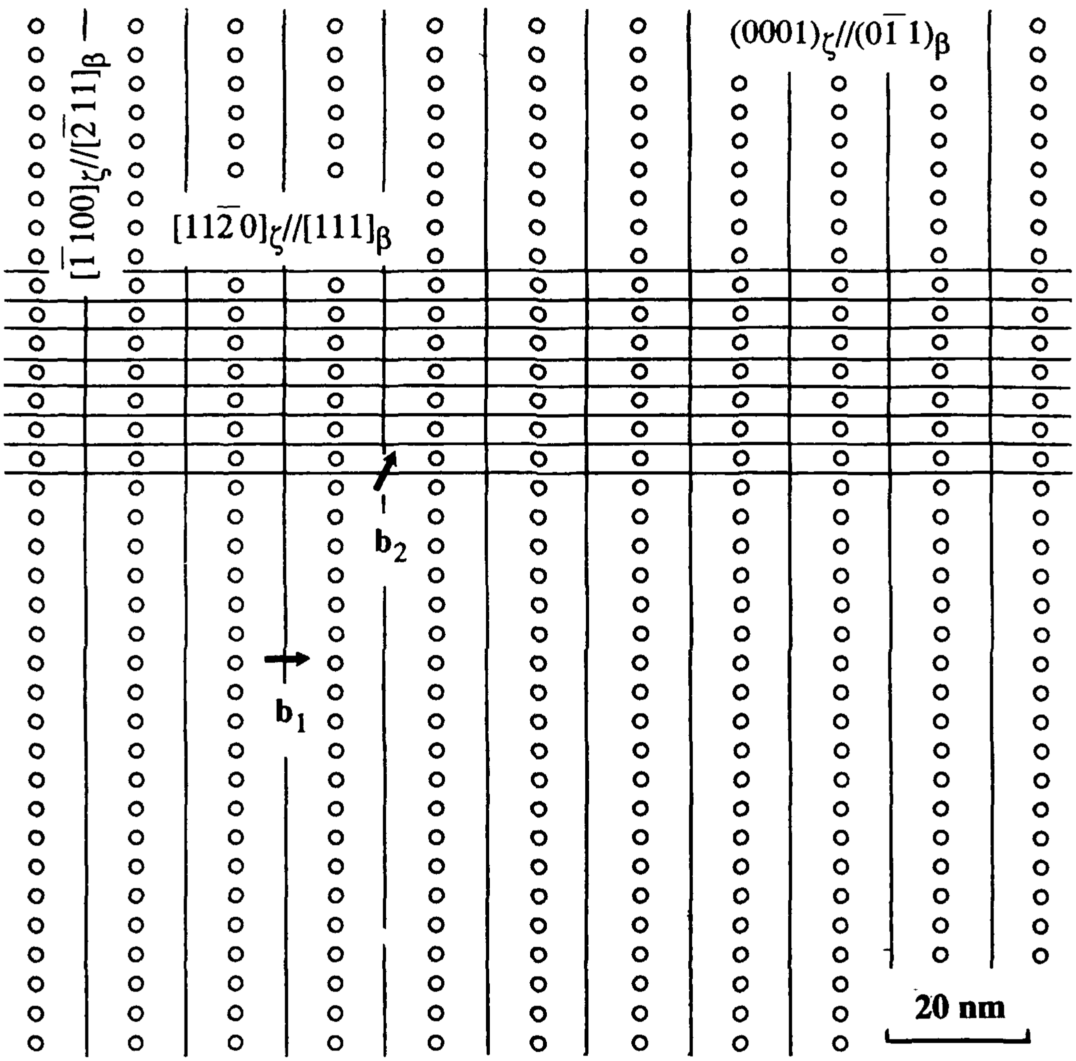


Figure 16



$[\bar{1}100]_\zeta // [\bar{2}11]_\beta$
$(0001)_\zeta // (0\bar{1}1)_\beta$
$[11\bar{2}0]_\zeta // [111]_\beta$
b_2
b_1
20 nm

Figure 17

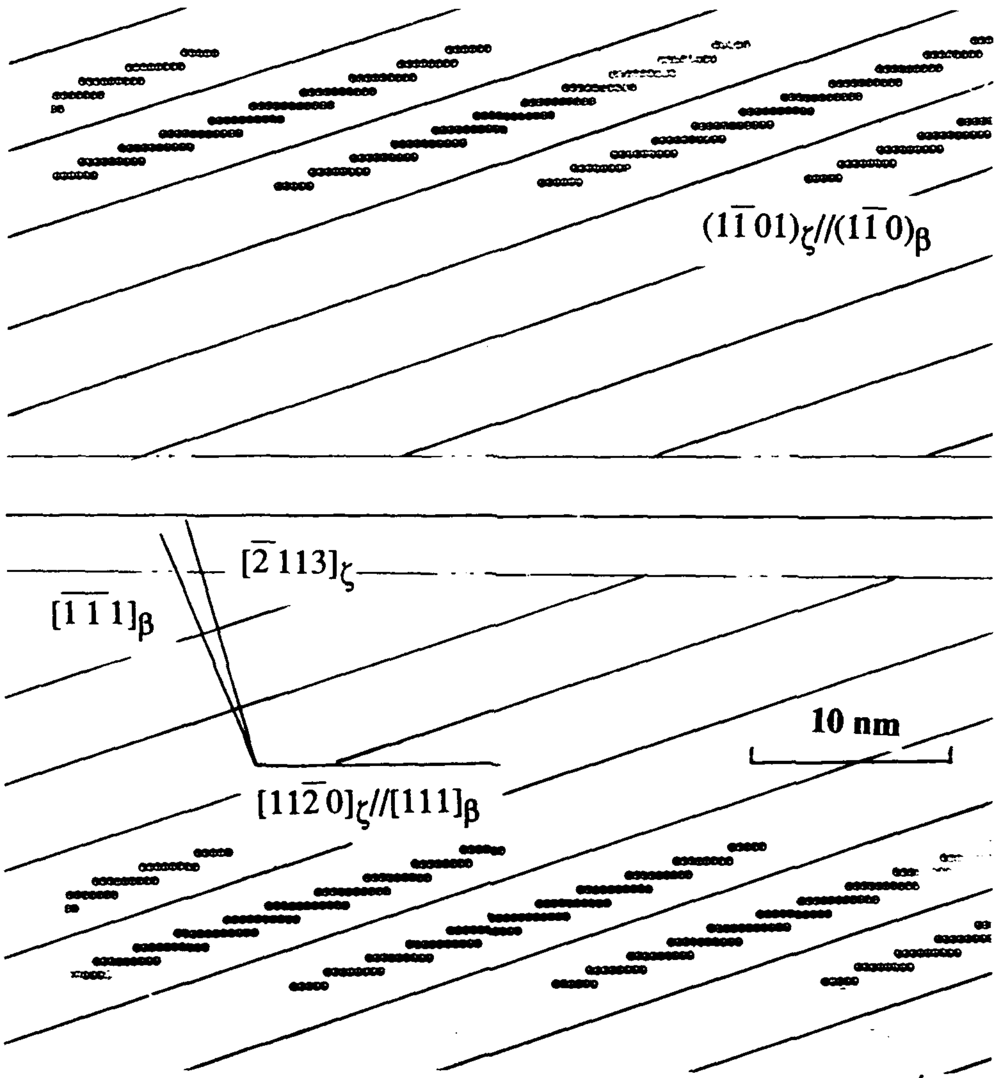
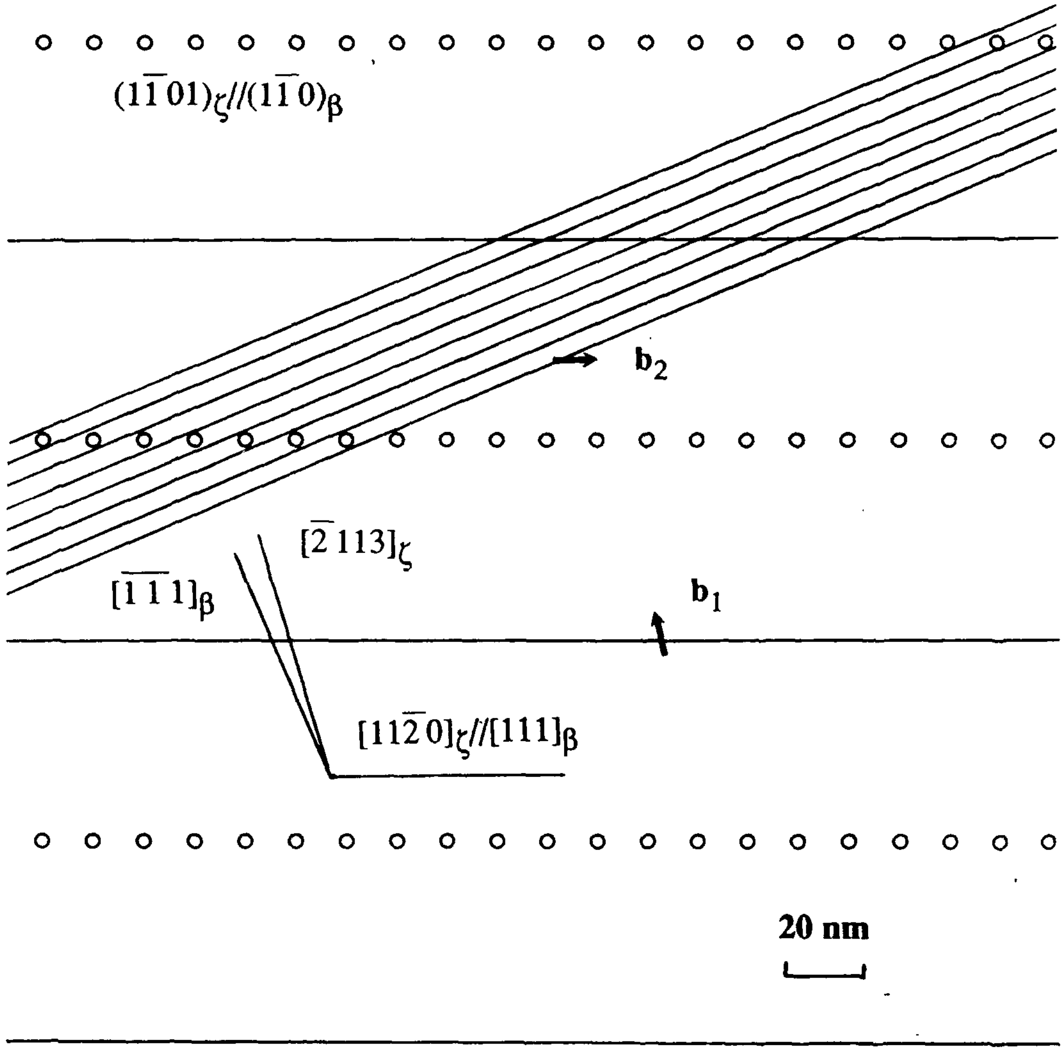


Figure 18



$(1\bar{1}01)_\zeta // (1\bar{1}0)_\beta$
$\mathbf{b}_2$
$[\bar{2}113]_\zeta$
$[\bar{1}\bar{1}1]_\beta$
$\mathbf{b}_1$
$[11\bar{2}0]_\zeta // [111]_\beta$
20 nm

Figure 19

Table I. Summary of Axis/Angle Pair Relationships - N-W OR

Dir'n (FCC)	Plane (FCC)	Combination	Axis/Angle (Calculated Directly)		Equivalent Axis/Angle	
			Angle	(BCC) Axis	Angle	(BCC) Axis
$a,\bar{b},\bar{c}$	111					
$\bar{b},\bar{c},a$	111	1+2	120°	$\overline{0.7071}$, 0.0, $\overline{0.7071}$	60°	0.7071, 0.0, 0.7071
$\bar{c},a,\bar{b}$	111	1+3	120°	0.7071, 0.0, 0.7071	60°	$\overline{0.7071}$, 0.0, $\overline{0.7071}$
$\bar{a},c,b$	$\bar{1}\bar{1}\bar{1}$	1+4	180°	$\overline{0.6124}$, 0.4999, 0.6124	60°	0.7071, 0.0, 0.7071
$b,\bar{a},c$	$\bar{1}\bar{1}\bar{1}$	1+5	180°	$\overline{0.6118}$, $\overline{0.5002}$, 0.6123	70.54°	0.7071, 0.0, 0.7071
$c,b,\bar{a}$	$\bar{1}\bar{1}\bar{1}$	1+6	180°	0.0000, 1.0000, 0.0000	0°	0.7071, 0.0, 0.7071
$a,\bar{c},b$	$11\bar{1}$	1+7	90°	$\overline{0.6961}$, $\overline{0.7072}$, $\overline{0.1197}$		
c,b,a	$11\bar{1}$	1+8	90°	$\overline{0.1691}$, $\overline{0.0002}$, 0.9856		
$\bar{b},a,c$	$11\bar{1}$	1+9	180°	0.3726, 0.4999, 0.7815		
$c,\bar{a},\bar{b}$	$\bar{1}\bar{1}1$	1+10	120°	0.0975, 0.8166, $\overline{0.5689}$		
b,c,a	$\bar{1}\bar{1}1$	1+11	120°	0.9024, 0.0002, $\overline{0.4310}$		
$a,\bar{b},c$	$\bar{1}\bar{1}1$	1+12	180°	0.6970, 0.7070, 0.1195		
$a,c,\bar{b}$	$1\bar{1}1$	1+13	90°	0.6961, 0.7072, 0.1197		
b,a,c	$1\bar{1}1$	1+14	90°	$\overline{0.6970}$, 0.7070, $\overline{0.1194}$		
$\bar{c},b,a$	$1\bar{1}1$	1+15	180°	0.9850, 0.0001, 0.1691		

a = 0.7291, b = 0.6828, c = 0.0463

Table II. Summary of Axis/Angle Pair Relationships - K-S OR

Dir'n (FCC)	Plane (FCC)	Combination	Axis/Angle (Calculated Directly) Angle	Axis/Angle (Calculated Directly) (BCC) Axis	Equivalent Axis/Angle Angle	Equivalent Axis/Angle (BCC) Axis
$1\overline{1}0$	111					
$\overline{1}01$	111	1+2	120°	$\overline{0.7071}$, 0.0, $\overline{0.7071}$	60°	0.7071, 0.0, 0.7071
$01\overline{1}$	111	1+3	120°	0.7071, 0.0, 0.7071	60°	$\overline{0.7071}$, 0.0, $\overline{0.7071}$
$\overline{1}01$	$\overline{111}$	1+4	180°	$\overline{0.6922}$, 0.4184, 0.6422	49.48°	0.7071, 0.0, 0.7071
$1\overline{1}0$	$\overline{111}$	1+5	180°	$\overline{0.5773}$, 0.5773, 0.5773	70.54°	0.7071, 0.0, 0.7071
$01\overline{1}$	$\overline{111}$	1+6	180°	$\overline{0.0649}$, 0.9958, 0.0649	10.59°	0.7071, 0.0, 0.7071
101	$11\overline{1}$	1+7	90°	$\overline{0.6498}$, $\overline{0.7415}$, $\overline{0.1667}$		
011	$11\overline{1}$	1+8	90°	$\overline{0.1667}$, $\overline{0.0749}$, $\overline{0.9832}$		
$\overline{1}10$	$11\overline{1}$	1+9	180°	0.3416, 0.4714, 0.8130	70.5°	$\overline{0.5773}$, $\overline{0.5773}$, 0.5773
$0\overline{11}$	$\overline{11}1$	1+10	120°	0.0432, 0.8563, $\overline{0.5147}$		
101	$\overline{11}1$	1+11	120°	0.8996, 0.0865, $\overline{0.4282}$		
$1\overline{1}0$	$\overline{11}1$	1+12	180°	0.7416, $\overline{0.6667}$, 0.0749		
$10\overline{1}$	$1\overline{1}1$	1+13	90°	0.6490, 0.7416, 0.1667		
110	$1\overline{1}1$	1+14	90°	$\overline{0.7415}$, 0.6667, $\overline{0.0749}$		
011	$1\overline{1}1$	1+15	180°	0.9838, 0.0529, 0.1708		

Table III. Summary of Axis/Angle Pair Relationships - Θ = 2°

Dir'n (FCC)	Plane (FCC)	Combination	Axis/Angle (Calculated Directly) Angle	Axis/Angle (Calculated Directly) (BCC) Axis	Equivalent Axis/Angle Angle	Equivalent Axis/Angle (BCC) Axis
$a,\bar{b},\bar{c}$	111					
$\bar{b},\bar{c},a$	111	1+2	120°	$\overline{0.7071}$, 0.0, $\overline{0.7071}$	60°	0.7071, 0.0, 0.7071
$\bar{c},a,\bar{b}$	111	1+3	120°	0.7071, 0.0, 0.7071	60°	$\overline{0.7071}$, 0.0, $\overline{0.7071}$
$\bar{a},c,b$	$\overline{111}$	1+4	180°	$\overline{0.6244}$, 0.4692, 0.6244	56°	0.7071, 0.0, 0.7071
$b,\bar{a},c$	$\overline{111}$	1+5	180°	0.5995, 0.5301, $\overline{0.5995}$	64°	0.7071, 0.0, 0.7071
$c,b,\bar{a}$	$\overline{111}$	1+6	180°	0.0248, $\overline{0.9993}$, $\overline{0.0248}$	4°	0.7071, 0.0, 0.7071
$a,\bar{c},b$	$11\bar{1}$	1+7	90°	$\overline{0.6796}$, $\overline{0.7210}$, $\overline{0.1373}$		
c,b,a	$11\bar{1}$	1+8	90°	$\overline{0.1687}$, $\overline{0.0086}$, 0.9852		
$\bar{b},a,c$	$11\bar{1}$	1+9	180°	0.3609, 0.4895, 0.7938		
$c,\bar{a},\bar{b}$	$\overline{111}$	1+10	120°	0.0771, 0.8325, $\overline{0.5485}$		
b,c,a	$\overline{111}$	1+11	120°	0.9019, 0.0331, $\overline{0.4306}$		
$a,\bar{b},c$	$\overline{111}$	1+12	180°	0.7413, $\overline{0.6923}$, 0.1022		
$a,c,\bar{b}$	$1\bar{1}1$	1+13	90°	0.6796, 0.7210, 0.1373		
b,a,c	$1\bar{1}1$	1+14	90°	$\overline{0.7143}$, 0.6923, $\overline{0.1022}$		
$\bar{c},b,a$	$1\bar{1}1$	1+15	180°	0.9853, 0.0203, 0.1694		

a = 0.7415, b = 0.6668, c = 0.0747

Table IV. Summary of Axis/Angle Pair Relationships - Watson & McDougall OR

Dir'n (FCC)	Plane (FCC)	Combination	Axis/Angle (Calculated Directly)		Equivalent Axis/Angle	
			Angle	(BCC) Axis	Angle	(BCC) Axis
$b,\overline{a},c$	h,k,e					
$\overline{a},c,b$	k,e,h	1+2	120°	$\overline{0.7084}$, 0.0201, $\overline{0.7055}$	60°	0.7071, 0.0, 0.7071
$c,b,\overline{a}$	ehk	1+3	120°	0.7084, $\overline{0.0203}$ 0.7055	60°	$\overline{0.7071}$, 0.0, $\overline{0.7071}$
$\overline{b},\overline{c},a$	$\overline{h\,e\,k}$	1+4	180°	$\overline{0.6371}$, 0.4119, 0.6515	48.66°	0.7071, 0.0, 0.7071
$a,\overline{b},\overline{c}$	$\overline{k\,h\,e}$	1+5	180°	0.5817, 0.5830, $\overline{0.5673}$	71.34°	0.7071, 0.0, 0.7071
$\overline{c},a,\overline{b}$	$\overline{e\,k\,h}$	1+6	180°	$\overline{0.0566}$, 0.9949 $\overline{0.0938}$	11.56°	0.7071, 0.0, 0.7071
$a,\overline{c},b$	$k,e,\overline{h}$	1+7	90°	$\overline{0.6500}$, $\overline{0.7415}$, $\overline{0.1667}$		
$\overline{c},a,b$	$e,k,\overline{h}$	1+8	90°	$\overline{0.1655}$, $\overline{0.0923}$, 0.9818		
$\overline{a},b,\overline{c}$	$k,h,\overline{e}$	1+9	180°	0.3476, 0.4525, 0.8213		
$\overline{c},\overline{b},\overline{a}$	$\overline{e},\overline{h},k$	1+10	120°	0.0502, 0.8656, $\overline{0.4908}$		
$a,\overline{c},b$	$\overline{k},\overline{e},h$	1+11	120°	0.8995, 0.0865, $\overline{0.4283}$		
$a,\overline{b},c$	$\overline{k},\overline{h},e$	1+12	180°	0.7355, $\overline{0.6748}$, 0.0605		
$b,\overline{c},\overline{a}$	$h,\overline{e},k$	1+13	90°	0.6571, 0.7322, 0.1796		
$a,b,\overline{c}$	$k,\overline{h},e$	1+14	90°	$\overline{0.7354}$, 0.6748, $\overline{0.0605}$		
$\overline{c},b,a$	$k,\overline{h},e$	1+15	180°	0.9827, 0.0394, 0.1818		

a = 0.7157, b = 0.6984, c = 0.0001, h = 0.5916, k = 0.5772, e = 0.5628

Table V. Observed and Calculated Contrast Behavior for a Potter OR Interface

g_{ζ_m}	Observed Contrast	$g \cdot b$ for 1/3 $[\bar{2}113]_{\zeta_m}$
0002	Strong	2
$11\bar{2}0$	Weak	-1
$10\bar{1}1$	None	0
$\bar{1}011$	Strong	2
$02\bar{2}0$	Very Weak	0
$01\bar{1}1$	Weak	1
$0\bar{1}11$	Weak	1

Table VI. Observed and Calculated Contrast Behavior for a Burgers OR Interface

g_{ζ_m}	Observed Contrast	$g \cdot b$ for $c[0001]_{\zeta_m}$
0002	Strong	2
$0\bar{1}11$	Weak	1
$11\bar{2}0$	Very Weak	0
$01\bar{1}1$	Weak	1
$02\bar{2}0$	None	0